

Design, synthesis, anticancer activity and mechanism studies of novel 2-amino-4-aryl-pyrimidine derivatives of ursolic acid

Wen-Yan Wang,^a Zi-Hui Yang,^a A-Liang Li,^a Qing-Song Liu,^a Yue Sun,^a
Wen Gu^{*a}

Fig. S1~Fig. S78. ¹H NMR, ¹³C NMR and HRMS spectra of
compounds 6a-j, 7a-j and 9a-f.

^a Jiangsu Provincial Key Lab for the Chemistry and Utilization of Agro-forest Biomass, Jiangsu Key Lab of Biomass-based Green Fuels and Chemicals, Co-Innovation Center for Efficient Processing and Utilization of Forest Products, College of Chemical Engineering, Nanjing Forestry University, Nanjing 210037, P. R. China.
E-mail address: njguwen@163.com.

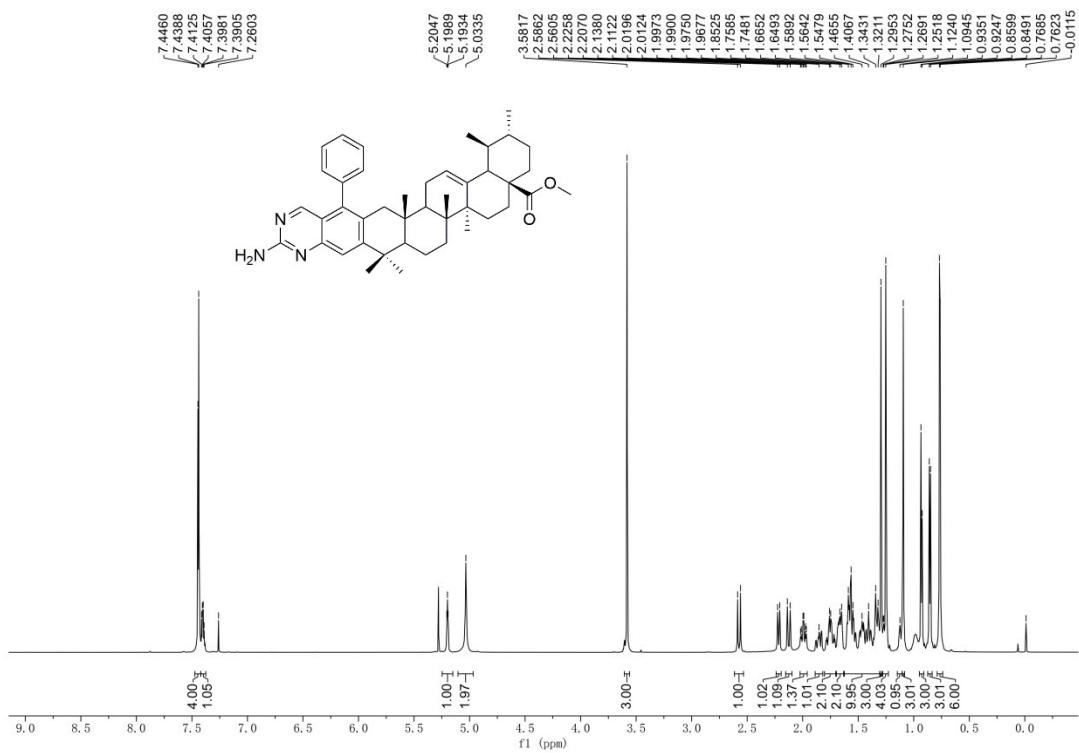


Fig. S1. ¹H NMR spectrum of compound 6a (600 MHz, CDCl₃)

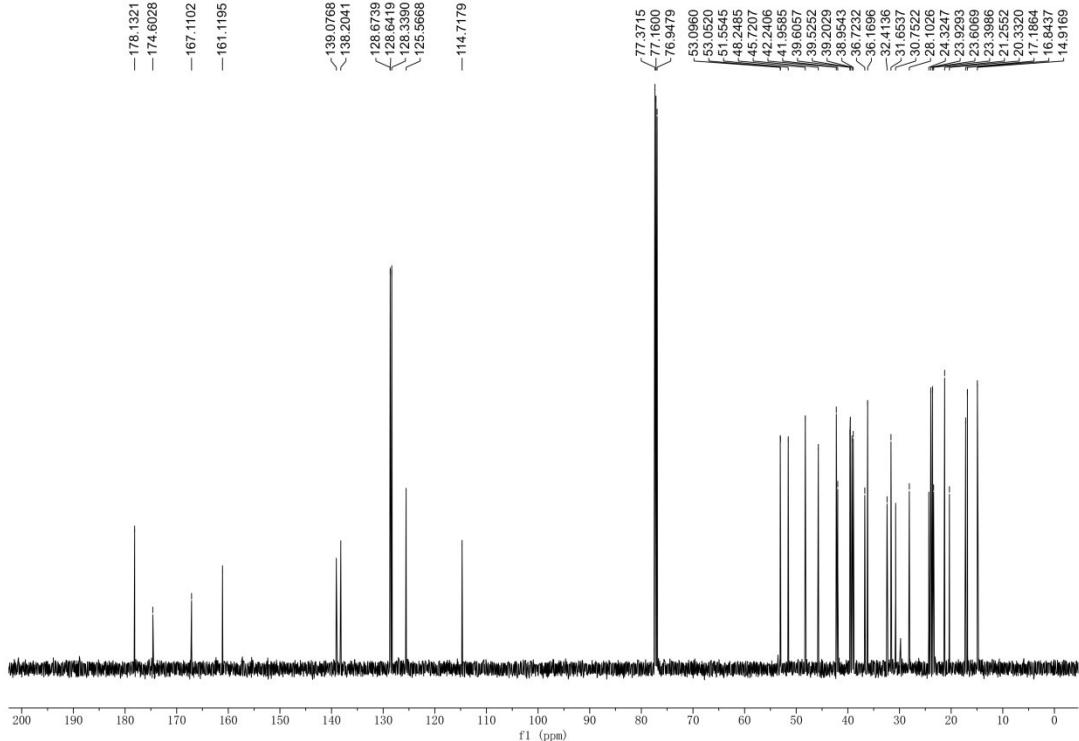


Fig. S2. ¹³C NMR spectrum of compound 6a (150 MHz, CDCl₃)

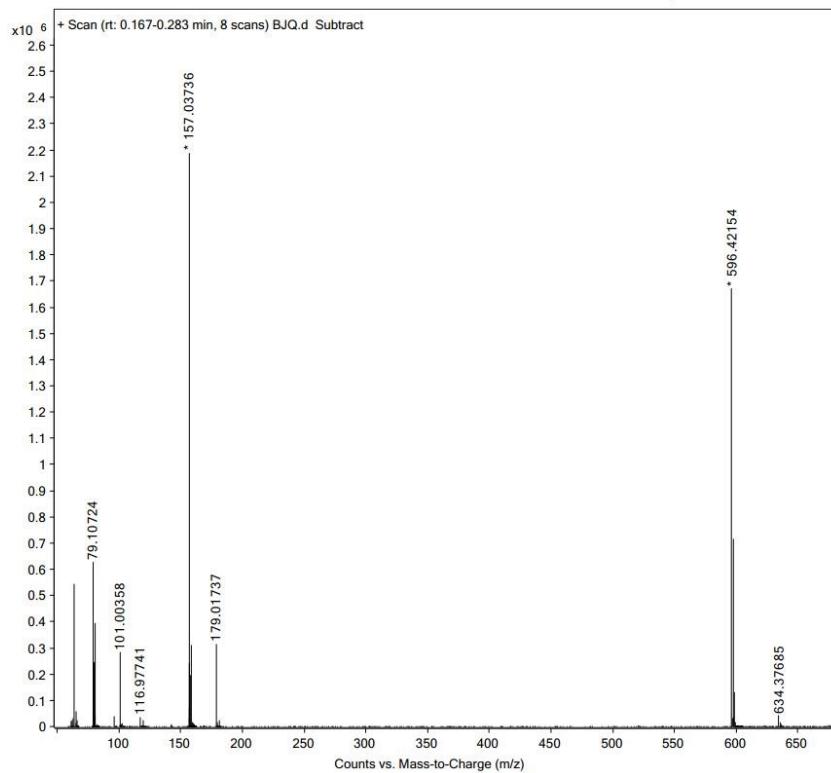


Fig. S3. HRMS spectrum of compound 6a

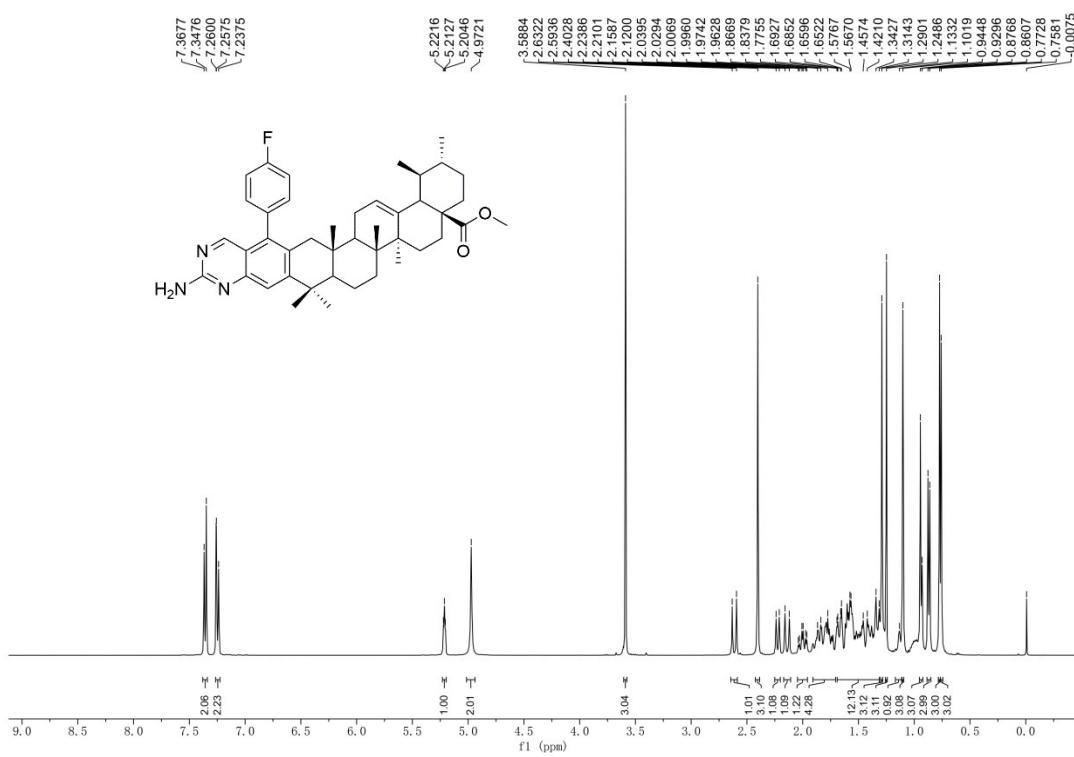


Fig. S4. ^1H NMR spectrum of compound 6b (600 MHz, CDCl_3)

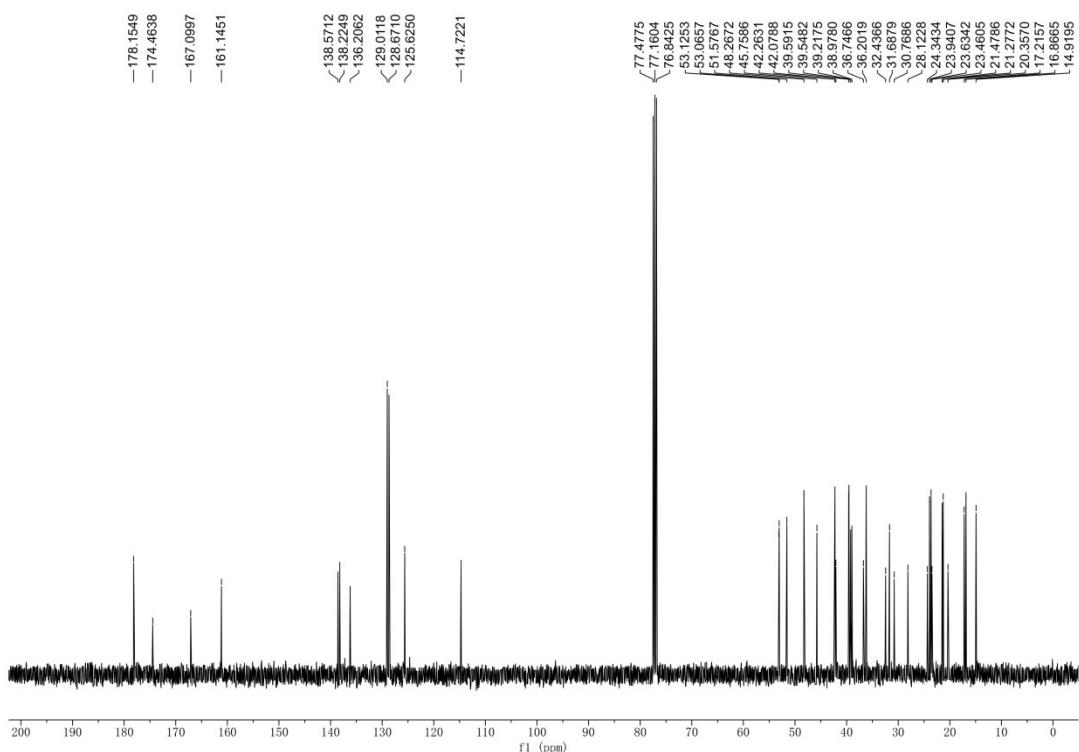


Fig. S5. ^{13}C NMR spectrum of compound 6b (150 MHz, CDCl_3)

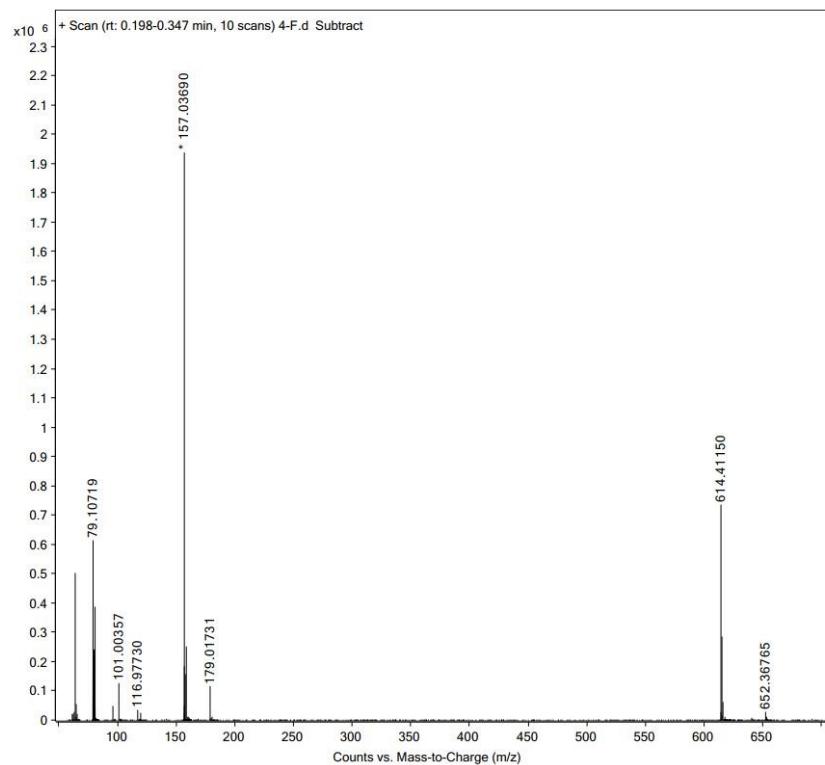


Fig. S6. HRMS spectrum of compound 6b

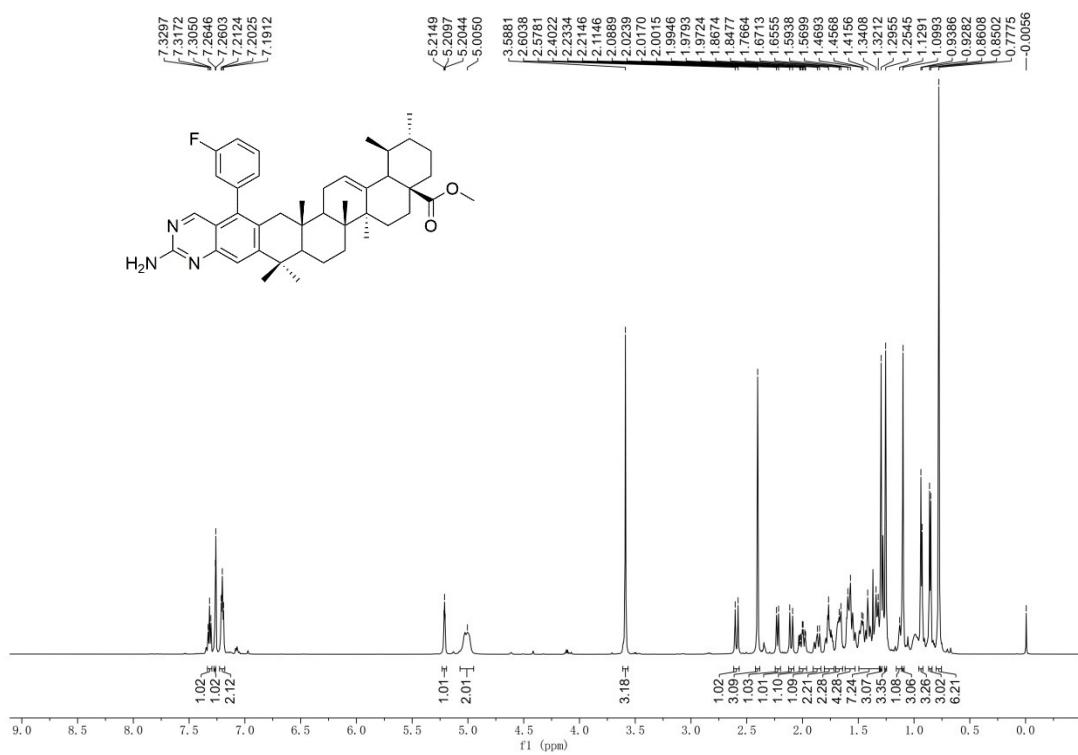


Fig. S7. ^1H NMR spectrum of compound 6c (600 MHz, CDCl_3)

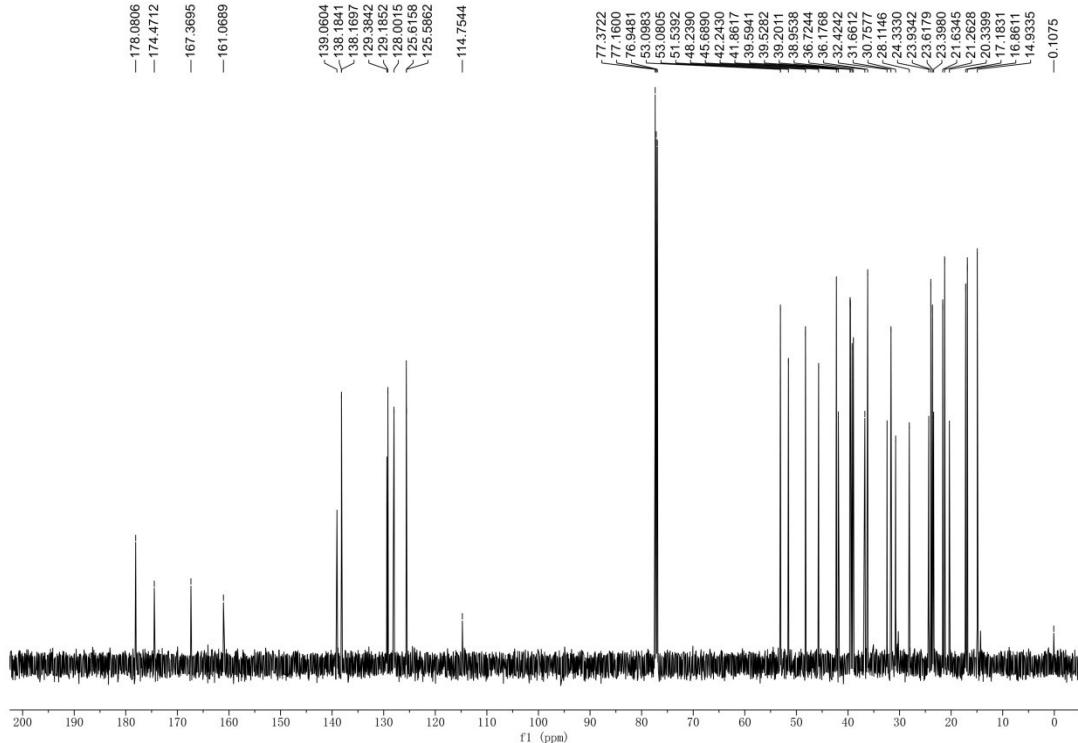


Fig. S8. ^{13}C NMR spectrum of compound 6c (150 MHz, CDCl_3)

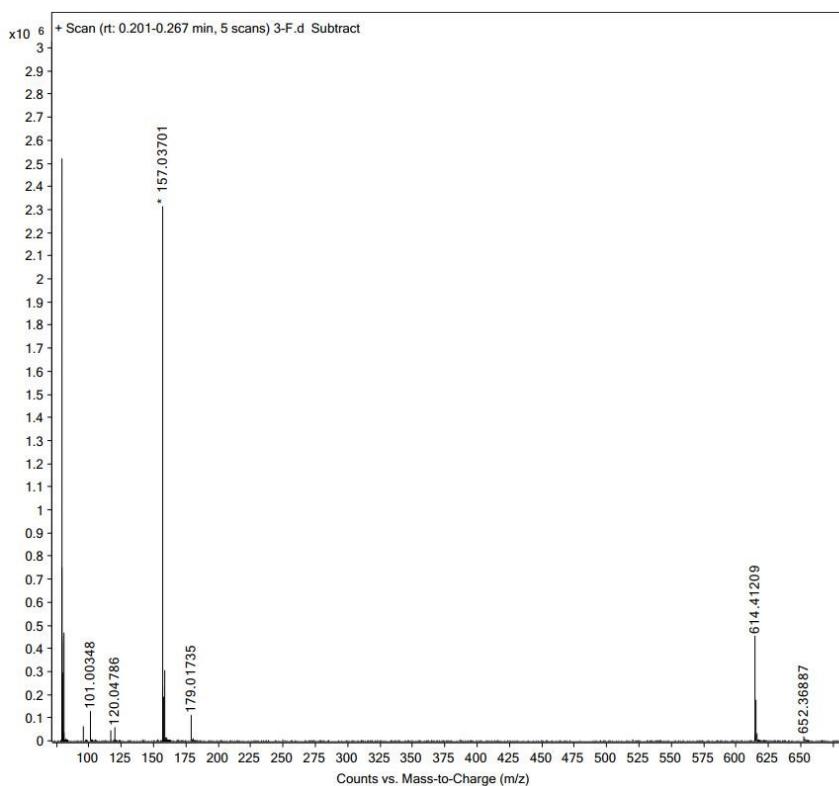


Fig. S9. HRMS spectrum of compound 6c

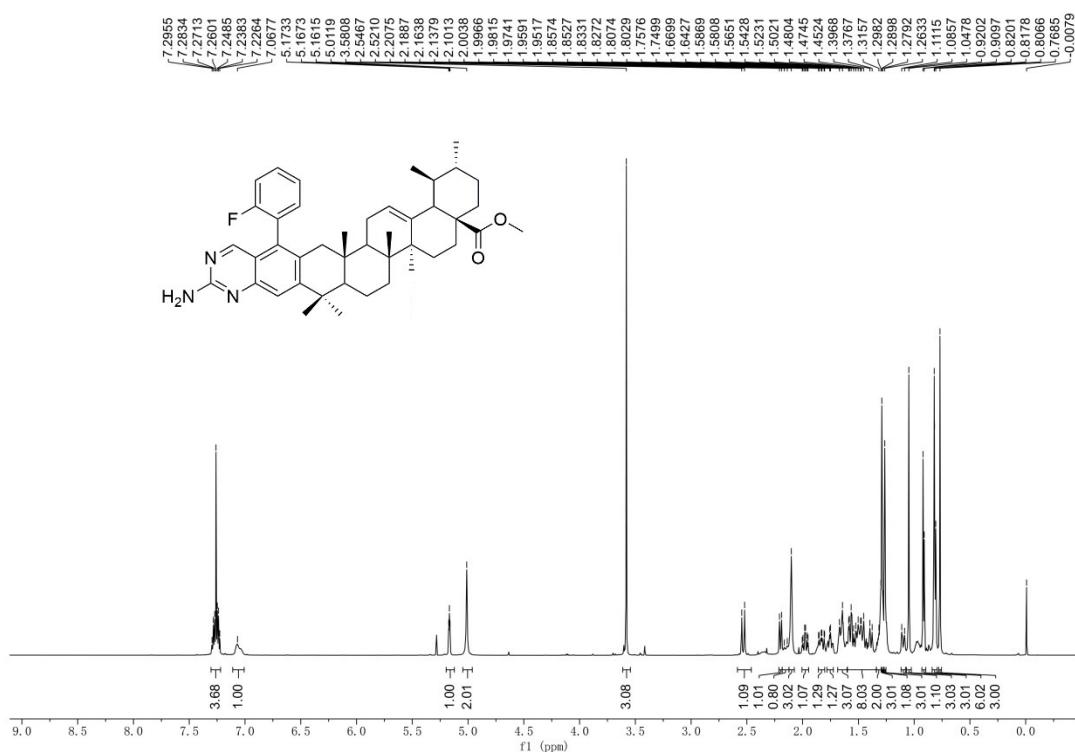


Fig. S10. ^1H NMR spectrum of compound 6d (600 MHz, CDCl_3)

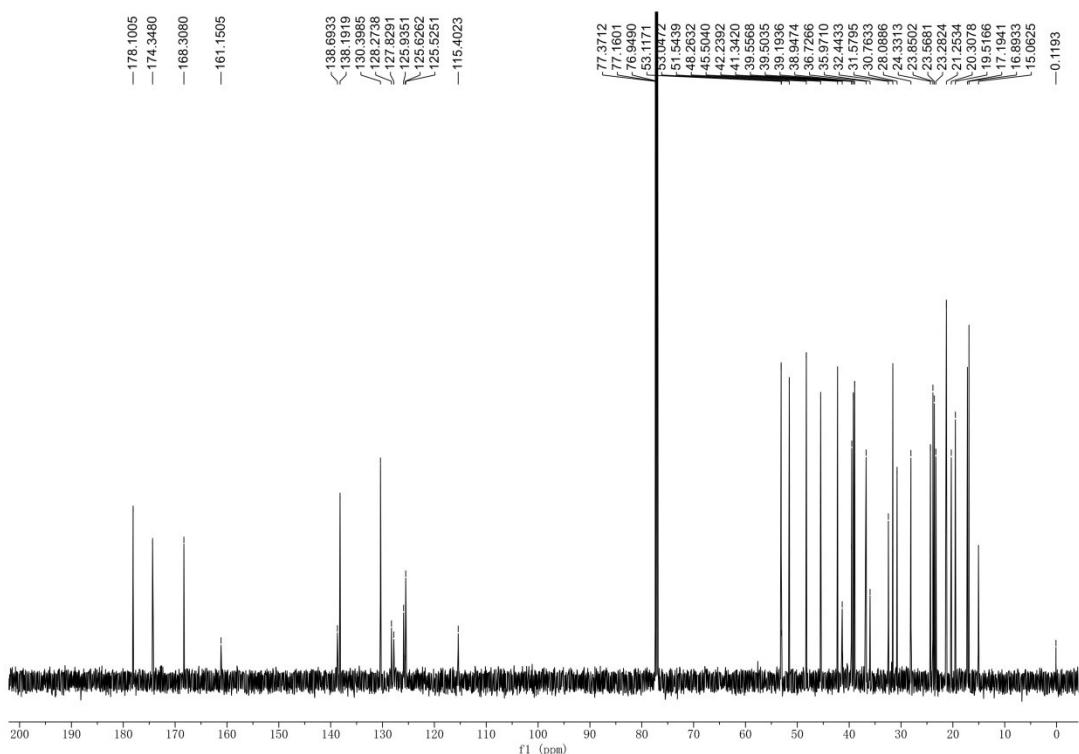


Fig. S11. ^{13}C NMR spectrum of compound 6d (150 MHz, CDCl_3)

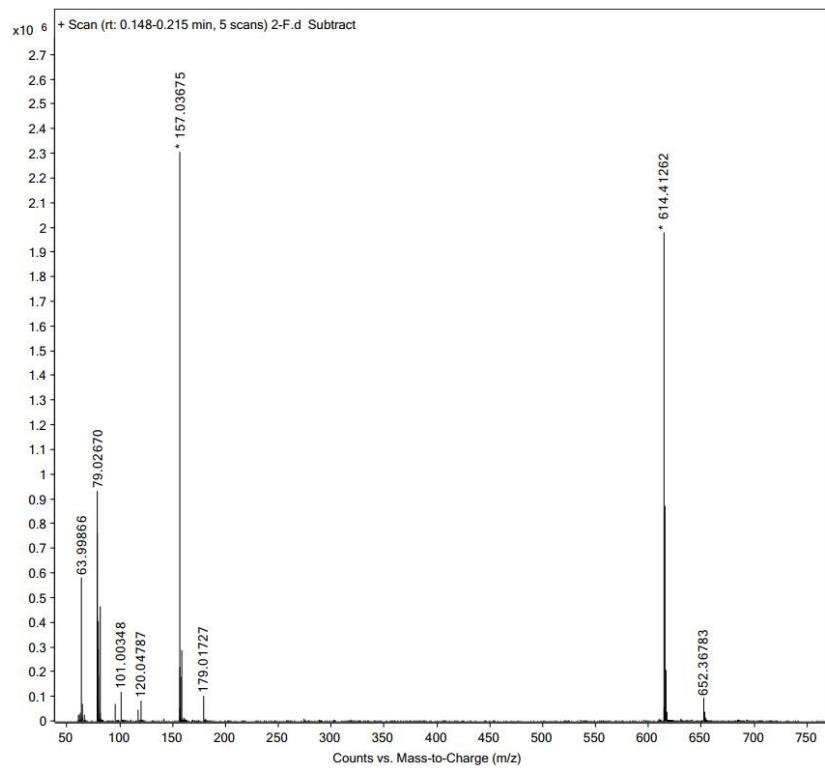


Fig. S12. HRMS spectrum of compound 6d

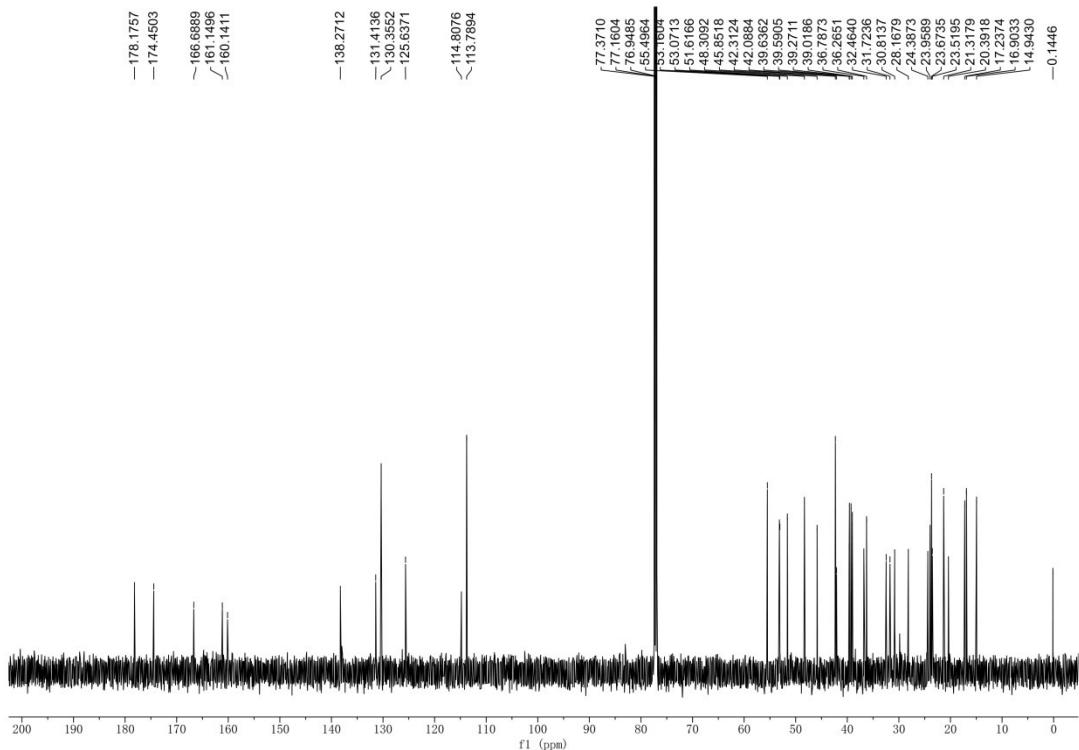
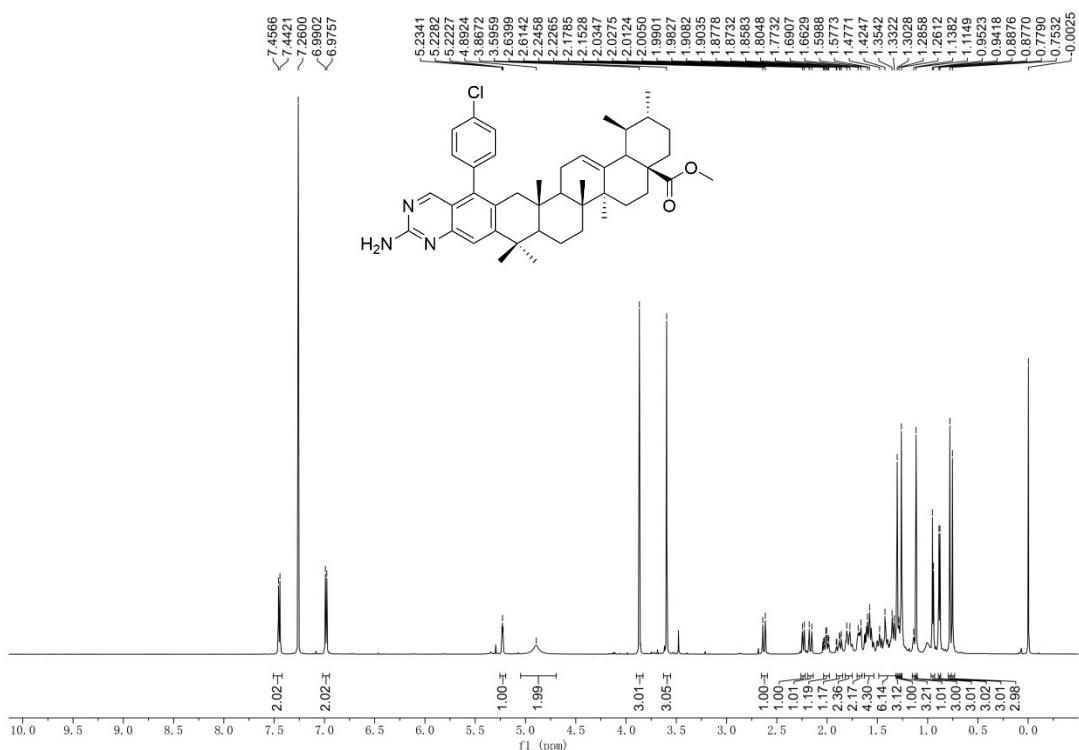


Fig. S14. ^{13}C NMR spectrum of compound 6e (150 MHz, CDCl_3)

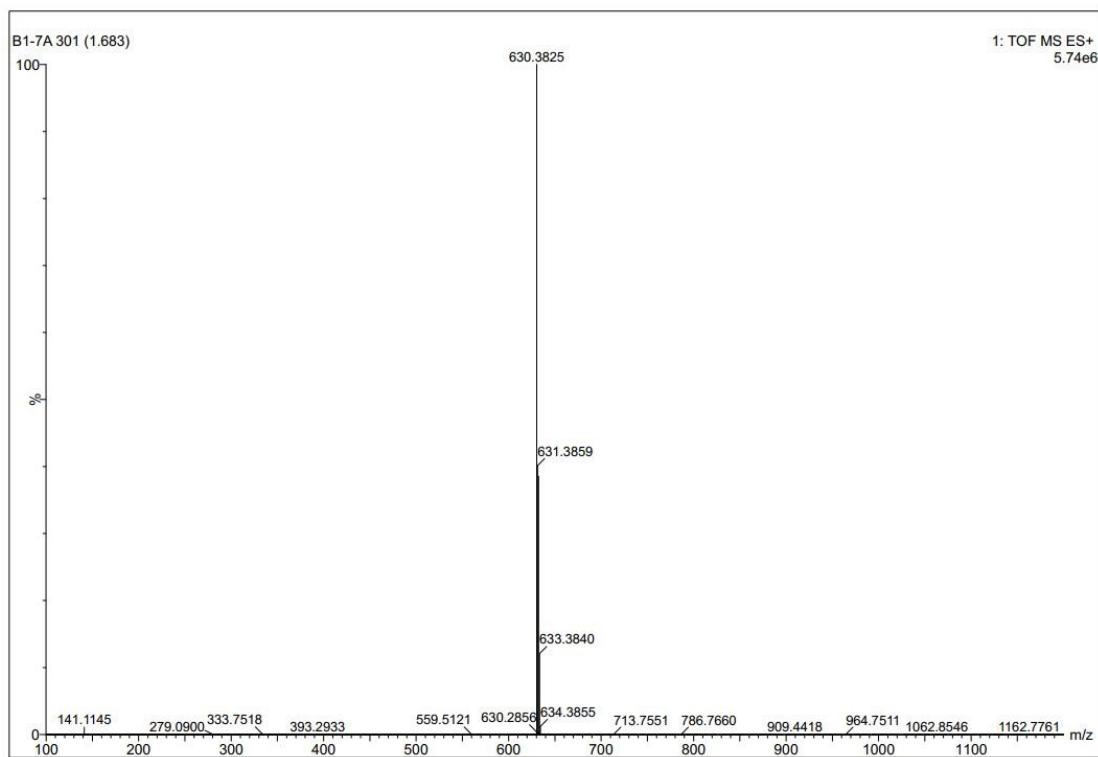


Fig. S15. HRMS spectrum of compound 6e

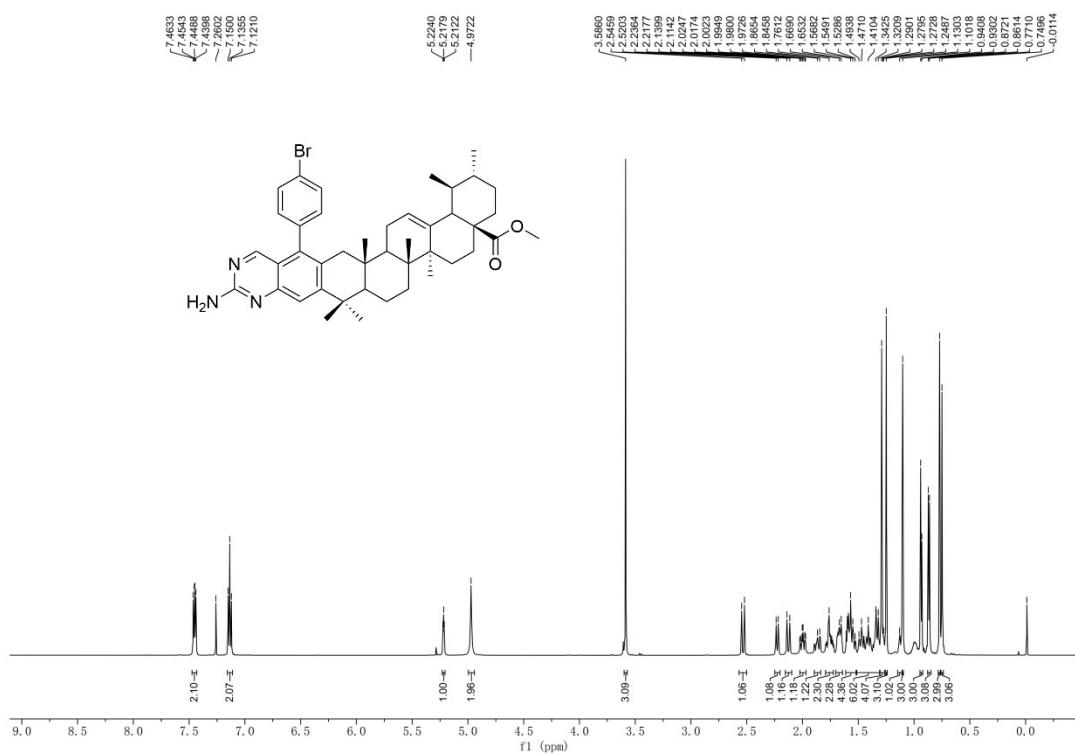


Fig. S16. ^1H NMR spectrum of compound 6f (600 MHz, CDCl_3)

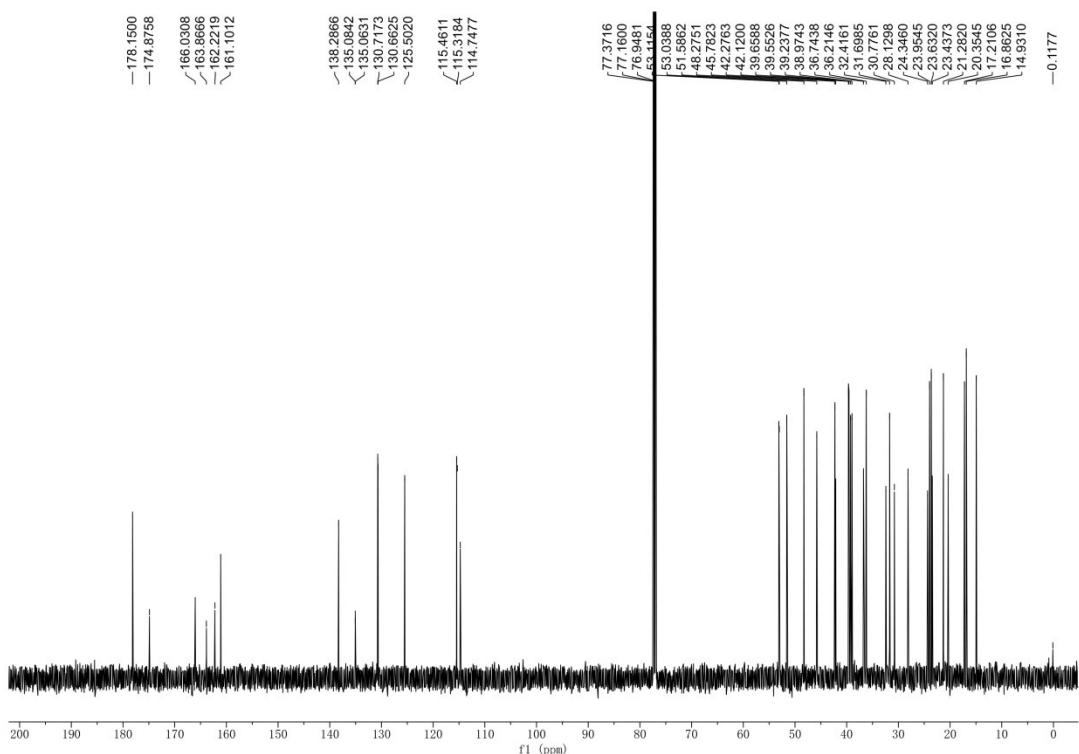


Fig. S17. ^{13}C NMR spectrum of compound 6f (150 MHz, CDCl_3)

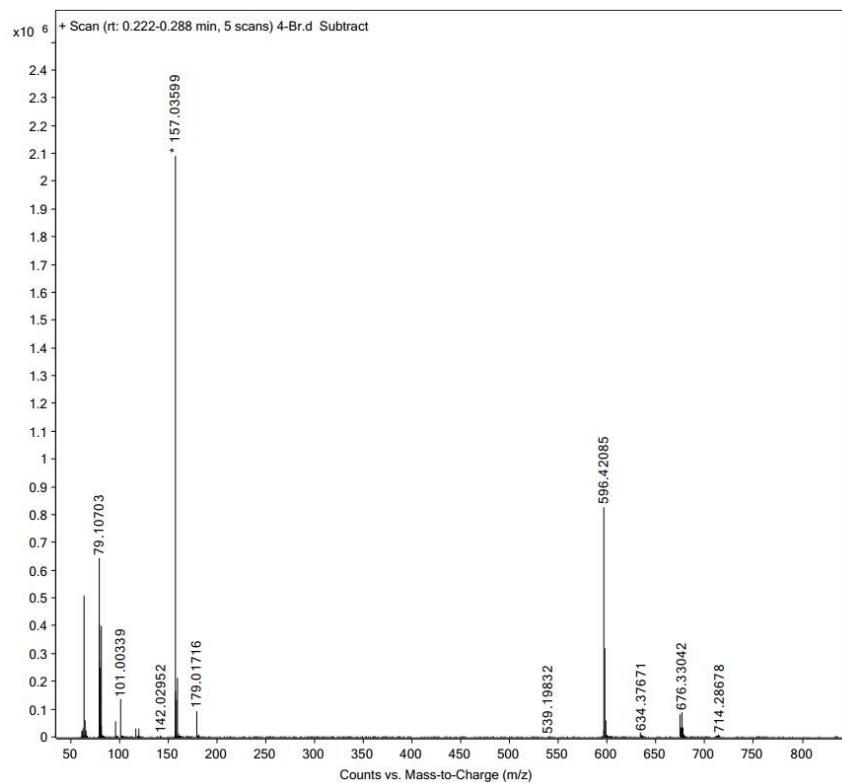


Fig. S18. HRMS spectrum of compound 6f

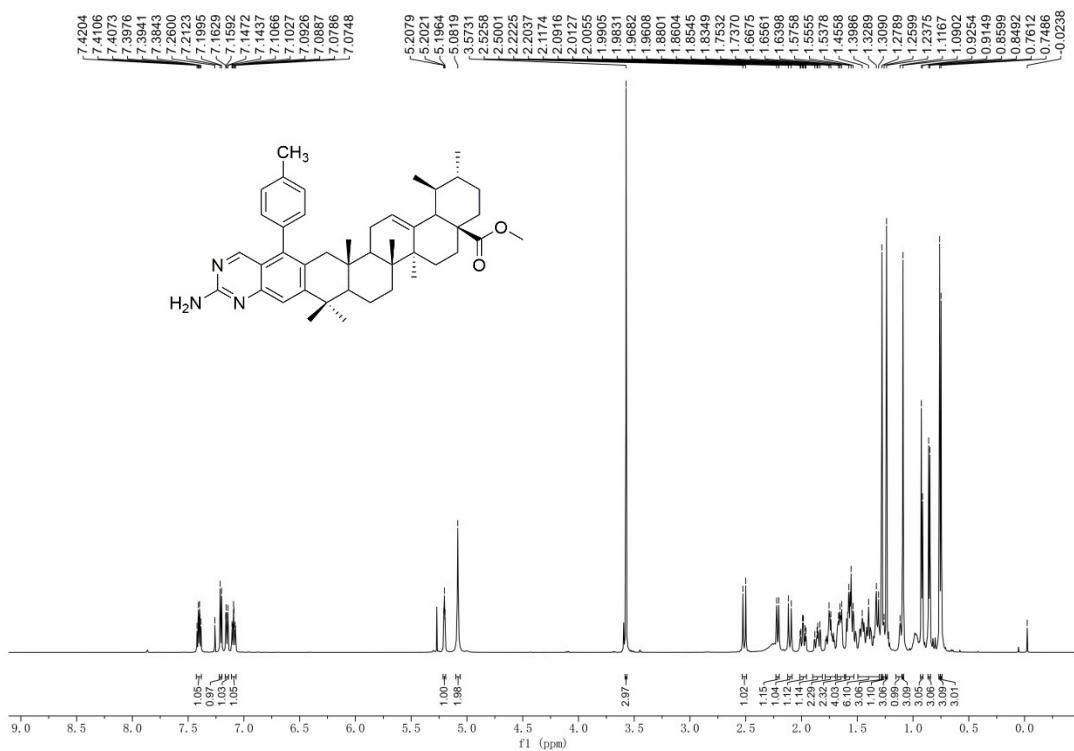


Fig. S19. ^1H NMR spectrum of compound 6g (600 MHz, CDCl_3)

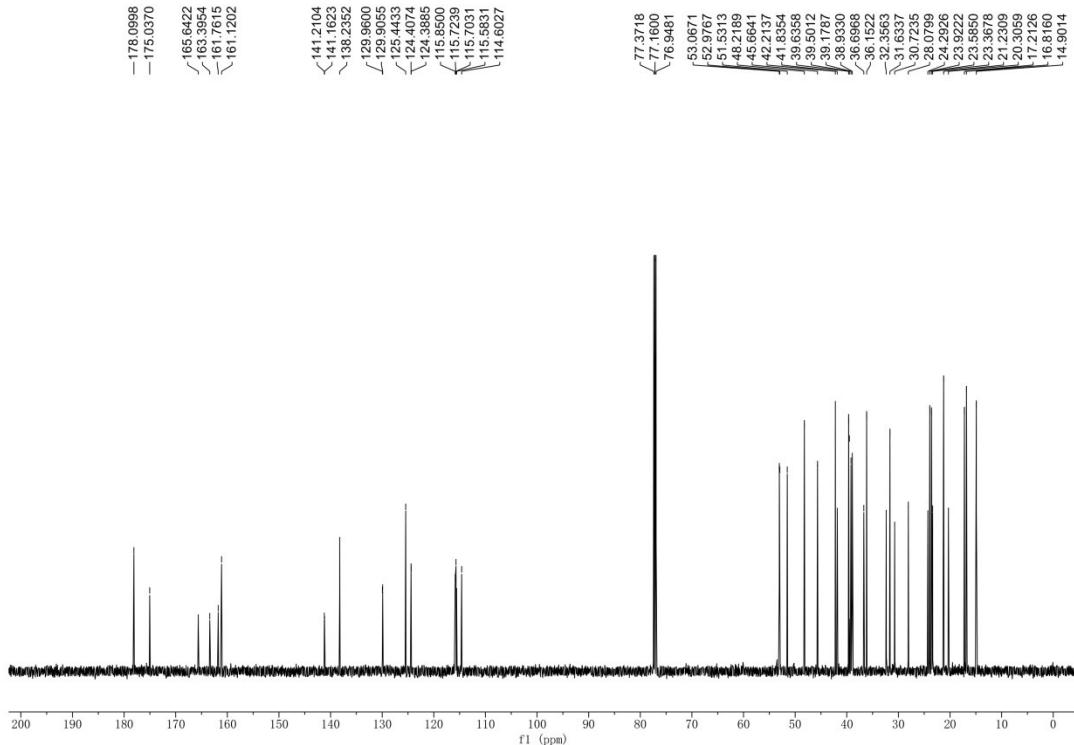


Fig. S20. ^{13}C NMR spectrum of compound 6g (150 MHz, CDCl_3)

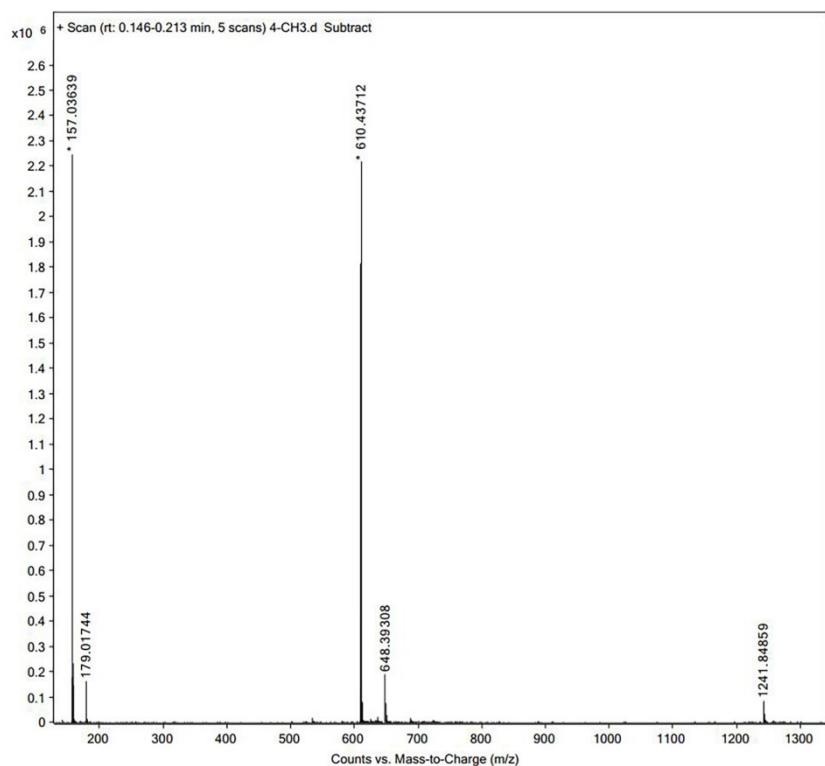


Fig. S21. HRMS spectrum of compound 6g

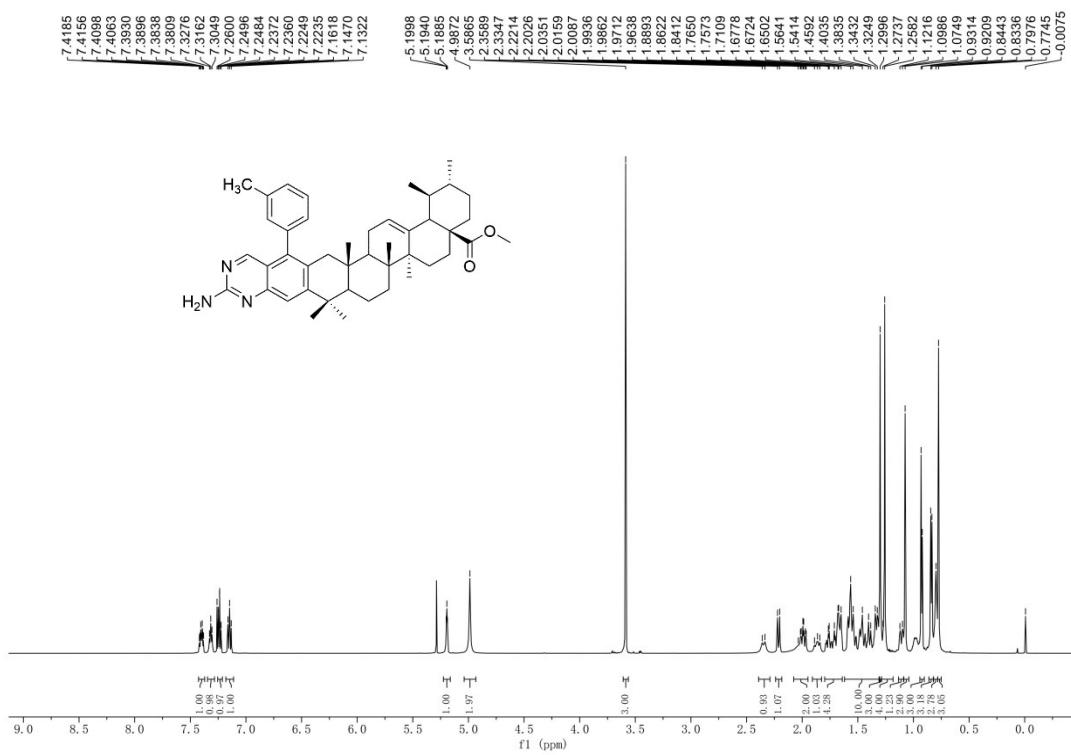


Fig. S22. ^1H NMR spectrum of compound 6h (600 MHz, CDCl_3)

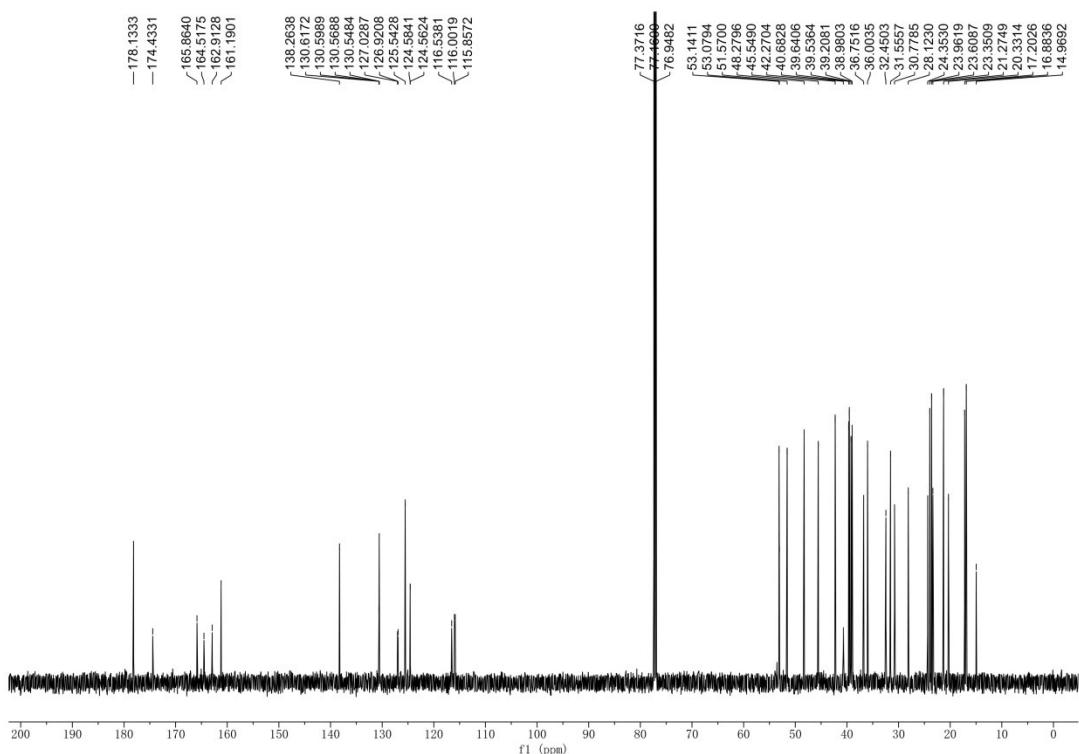


Fig. S23. ^{13}C NMR spectrum of compound 6h (150 MHz, CDCl_3)

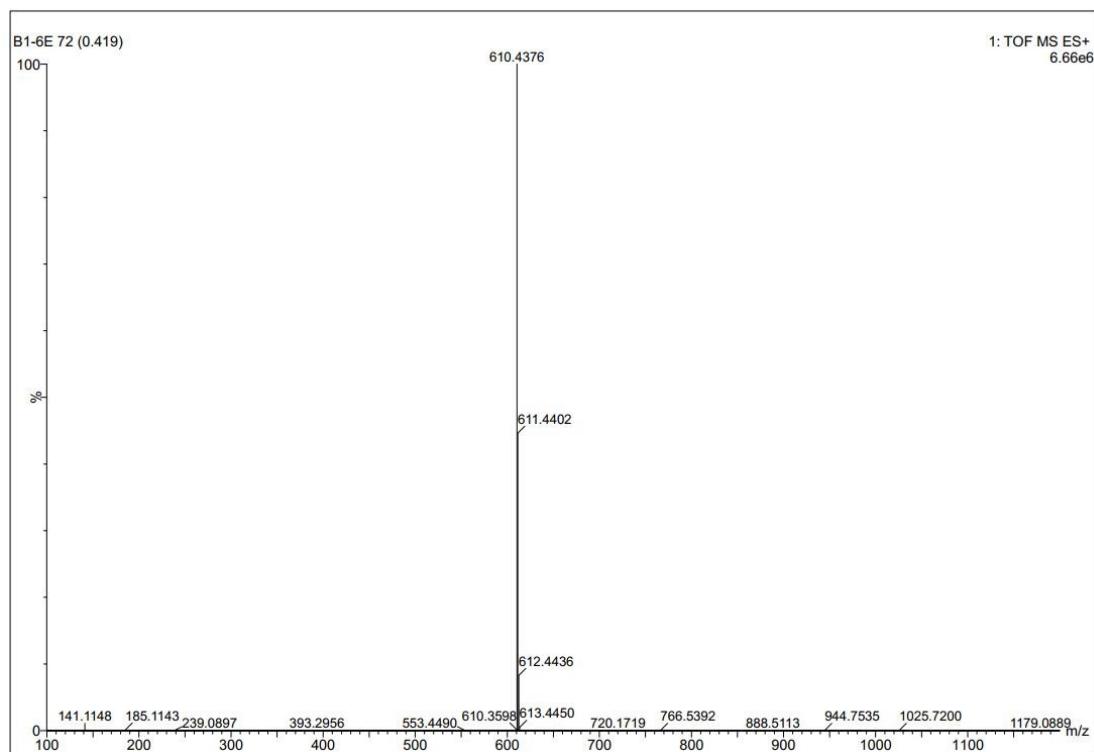


Fig. S24. HRMS spectrum of compound 6h

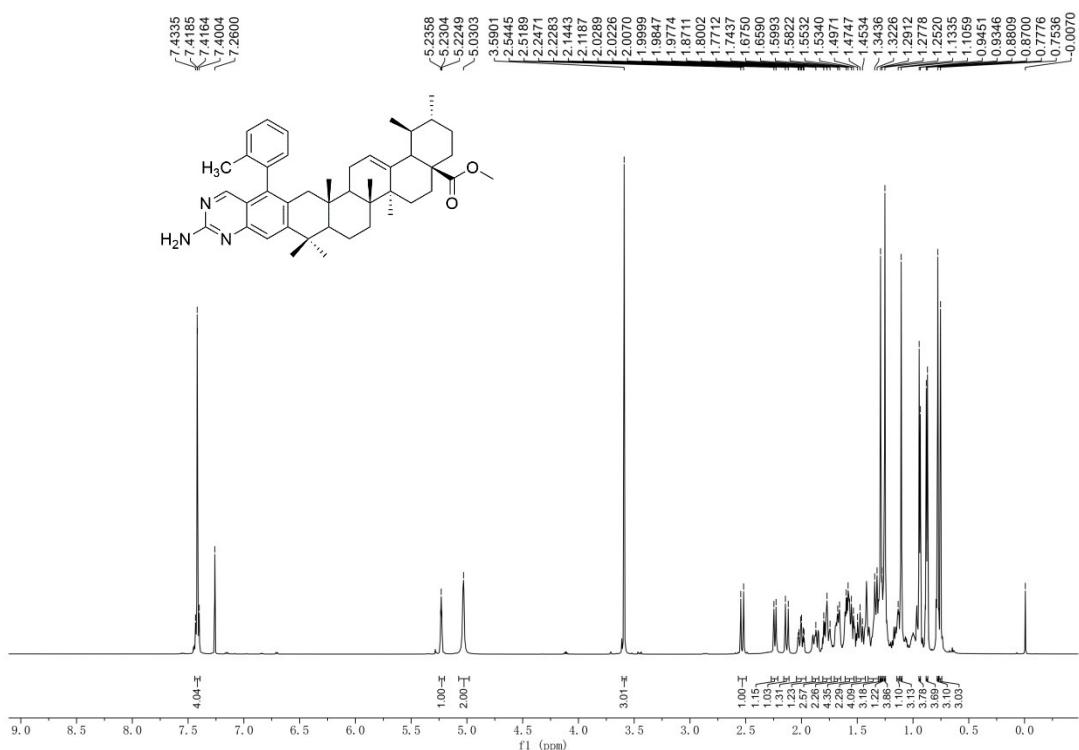


Fig. S25. ¹H NMR spectrum of compound 6i (600 MHz, CDCl₃)

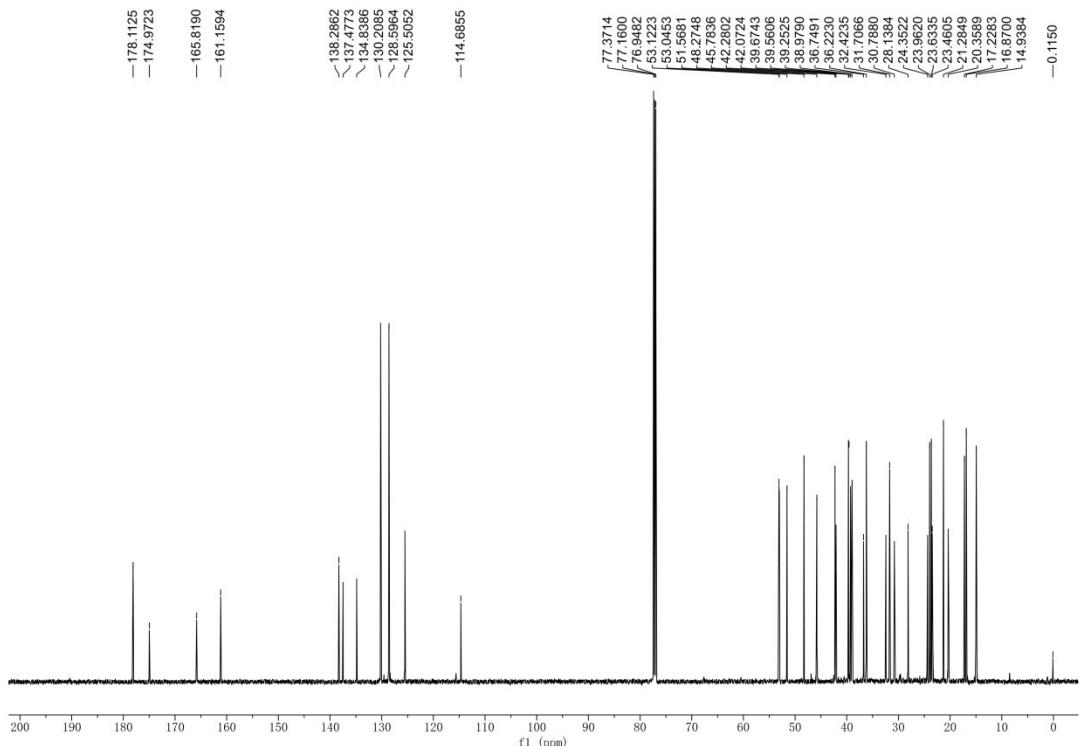


Fig. S26. ¹³C NMR spectrum of compound 6i (150 MHz, CDCl₃)

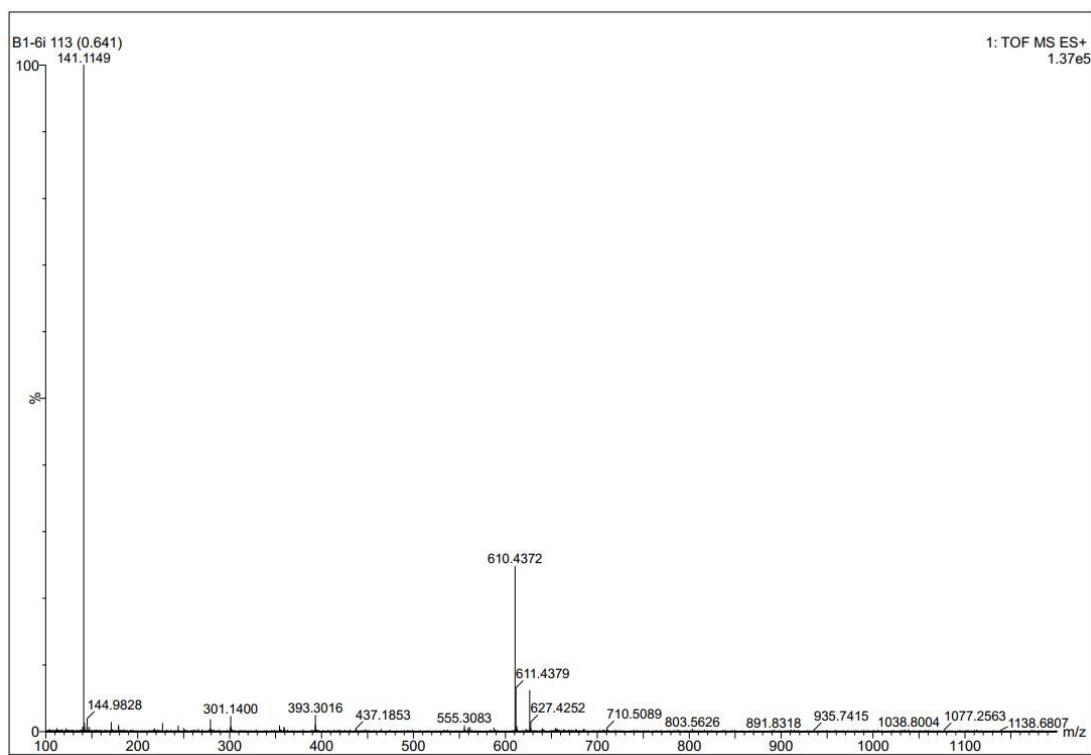


Fig. S27. HRMS spectrum of compound 6i

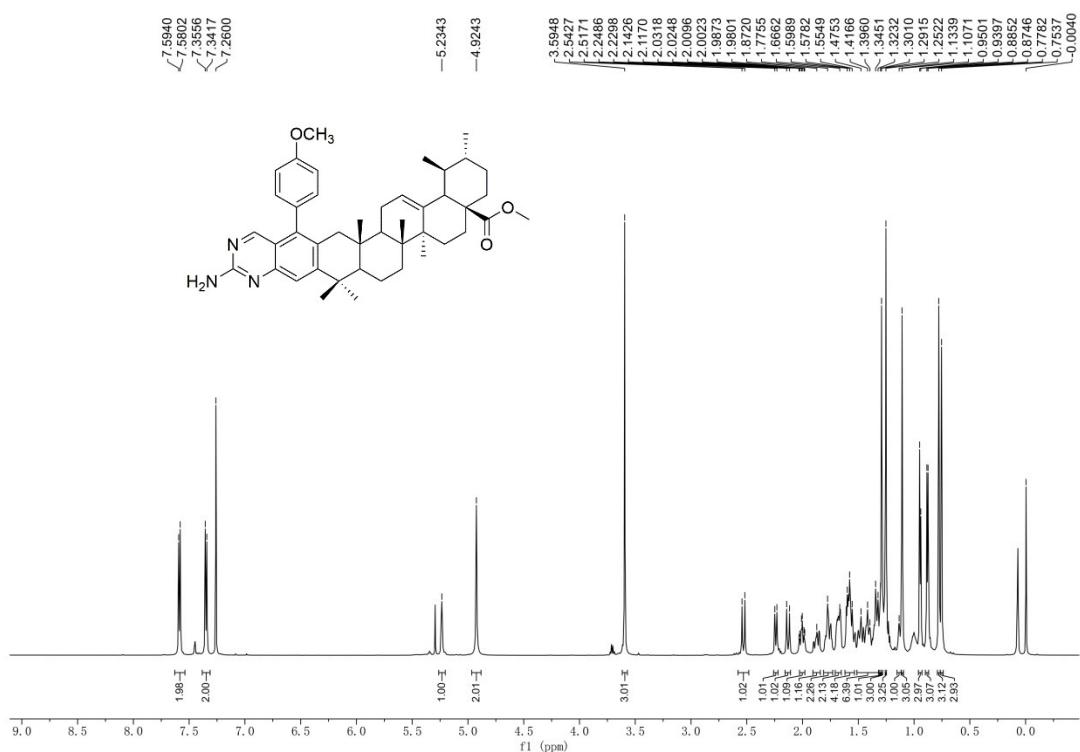


Fig. S28. ¹H NMR spectrum of compound 6j (600 MHz, CDCl₃)

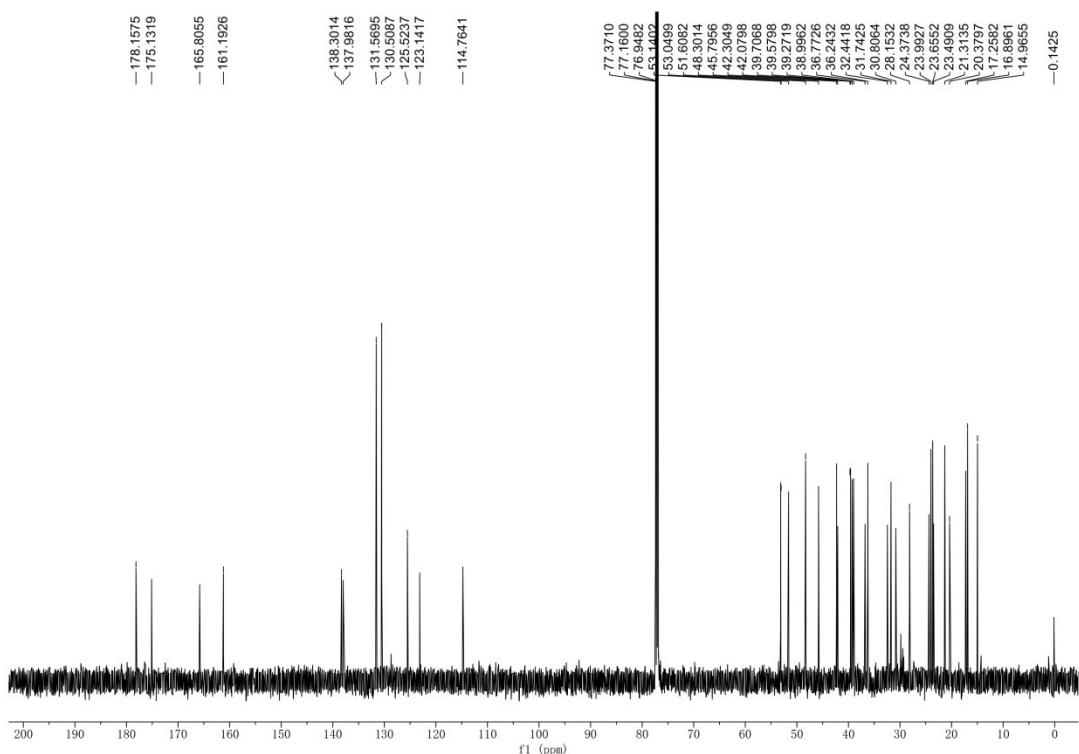


Fig. S29. ^{13}C NMR spectrum of compound 6j (150 MHz, CDCl_3)

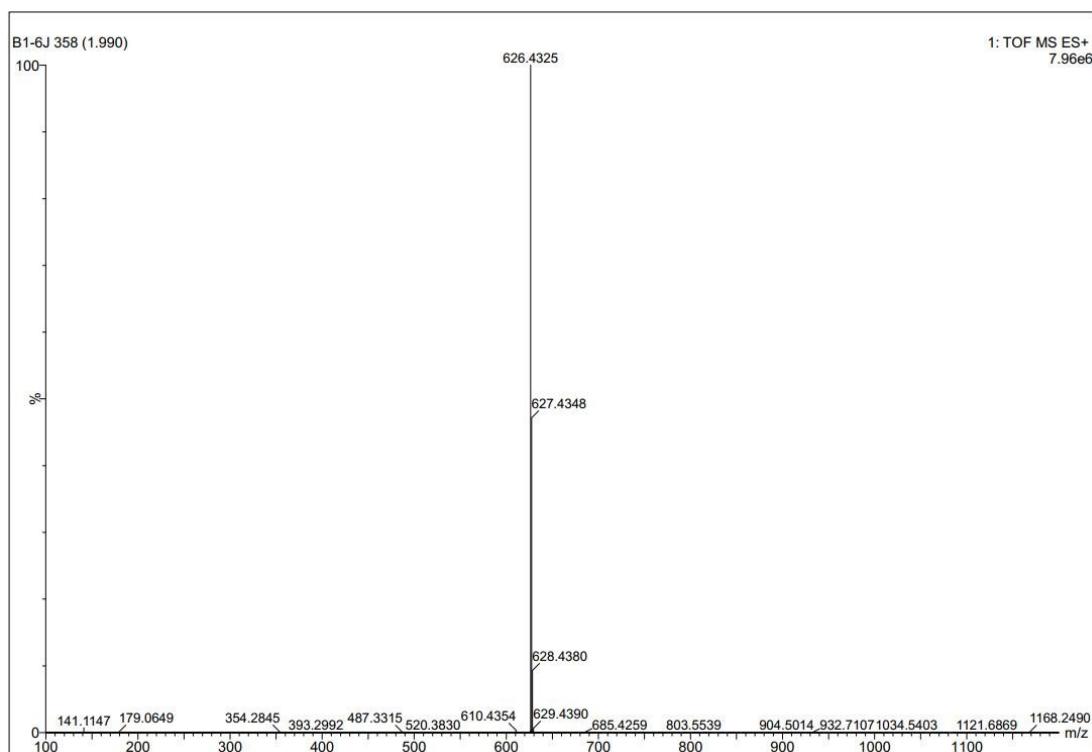


Fig. S30. HRMS spectrum of compound 6j

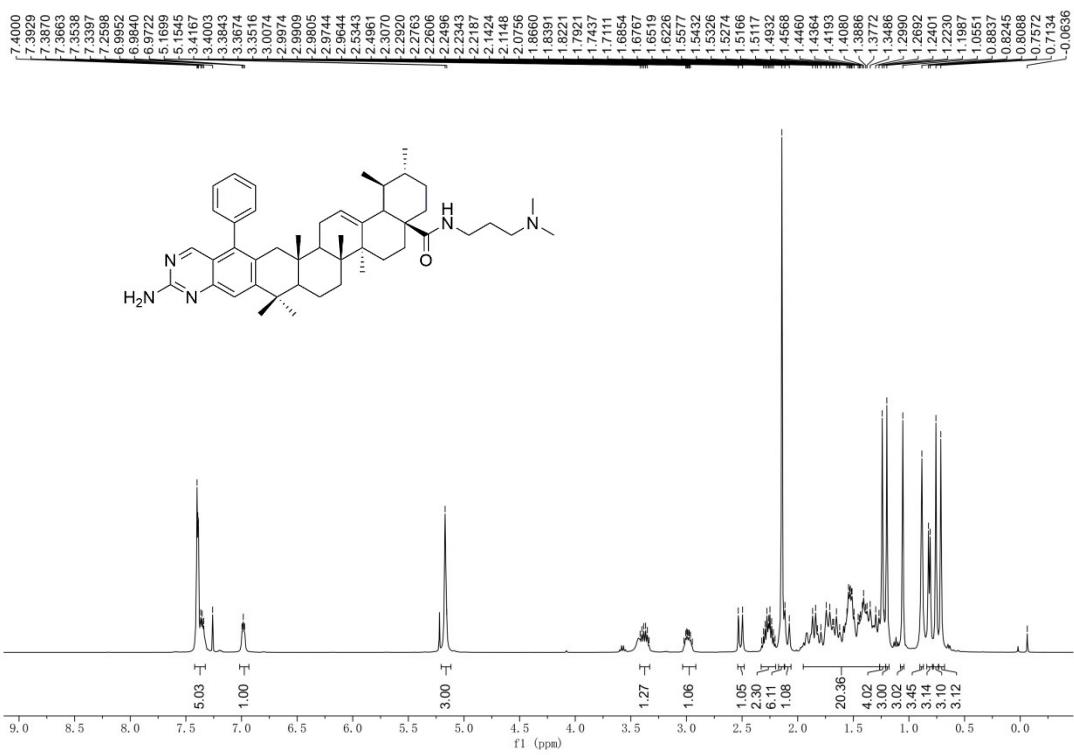


Fig. S31. ¹H NMR spectrum of compound 7a (600 MHz, CDCl₃)

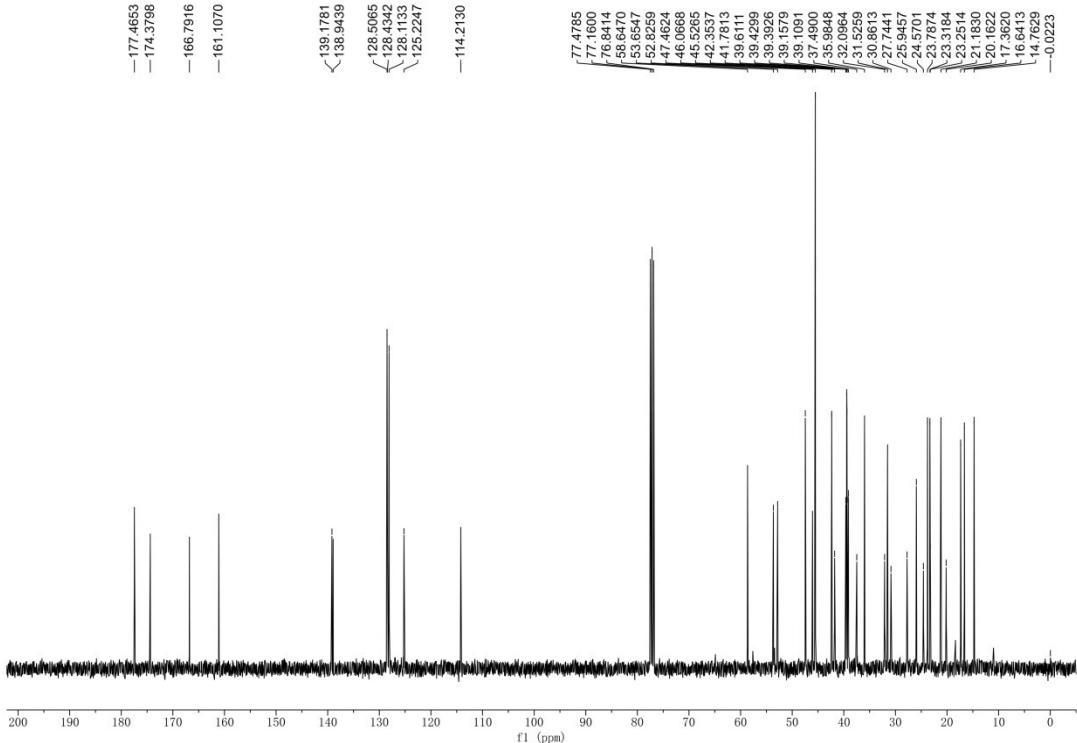


Fig. S32. ¹³C NMR spectrum of compound 7a (150 MHz, CDCl₃)

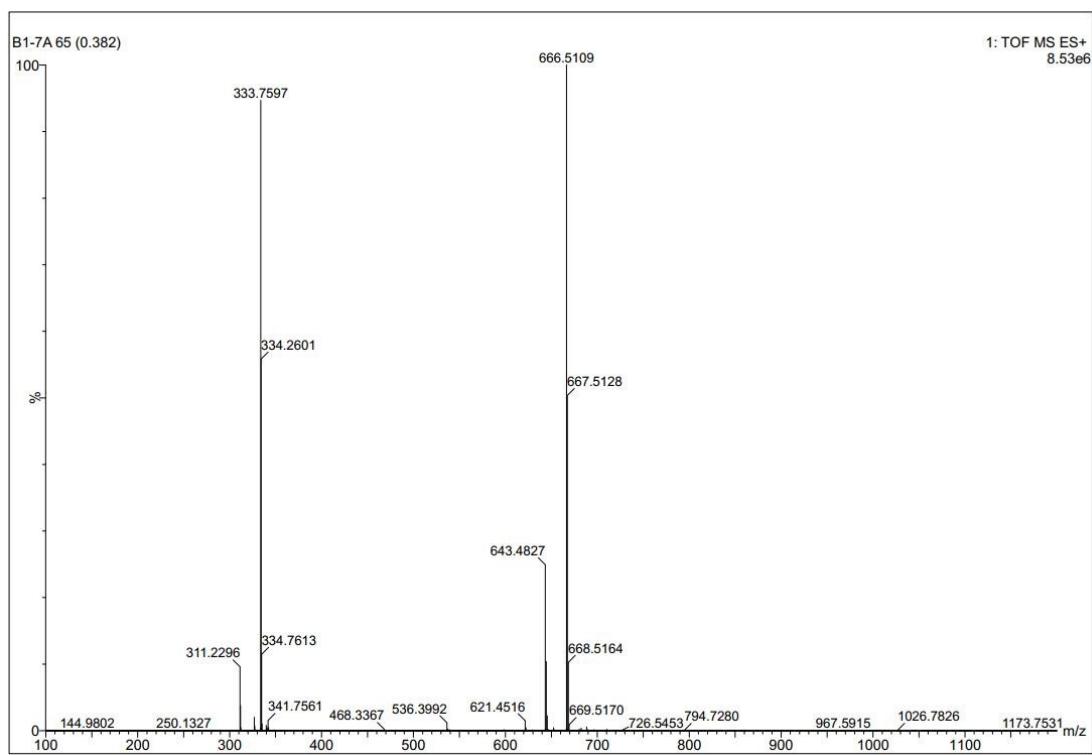


Fig. S33. HRMS spectrum of compound 7a

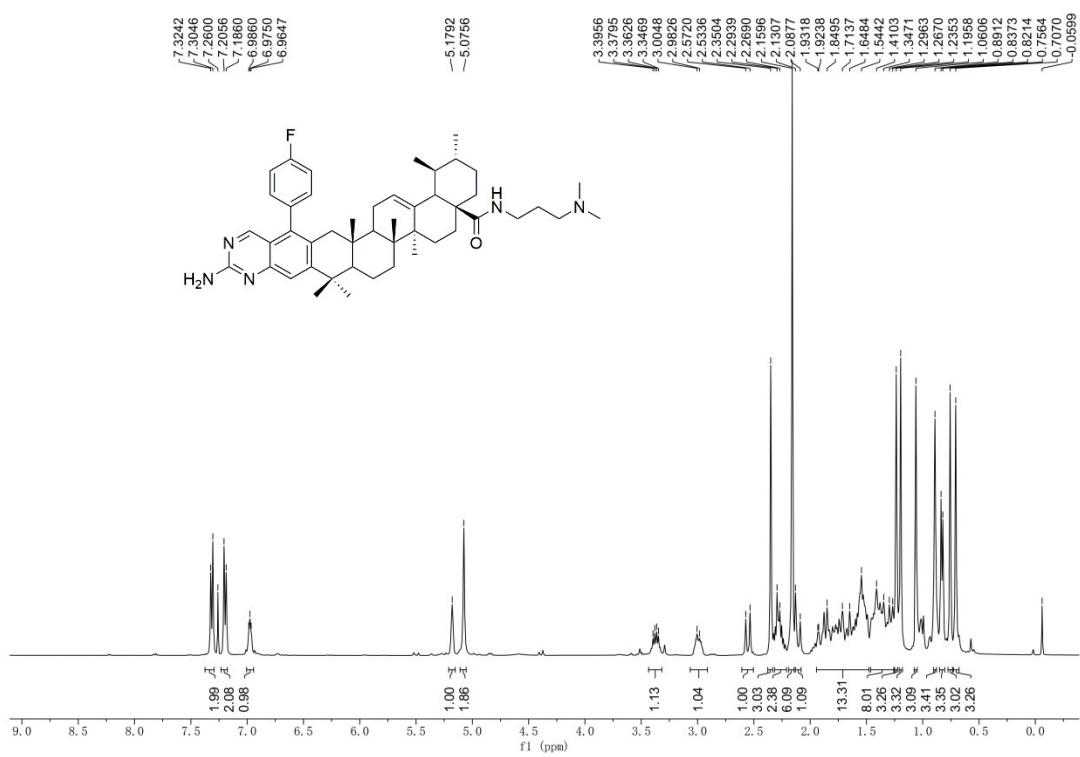


Fig. S34. ¹H NMR spectrum of compound 7b (600 MHz, CDCl₃)

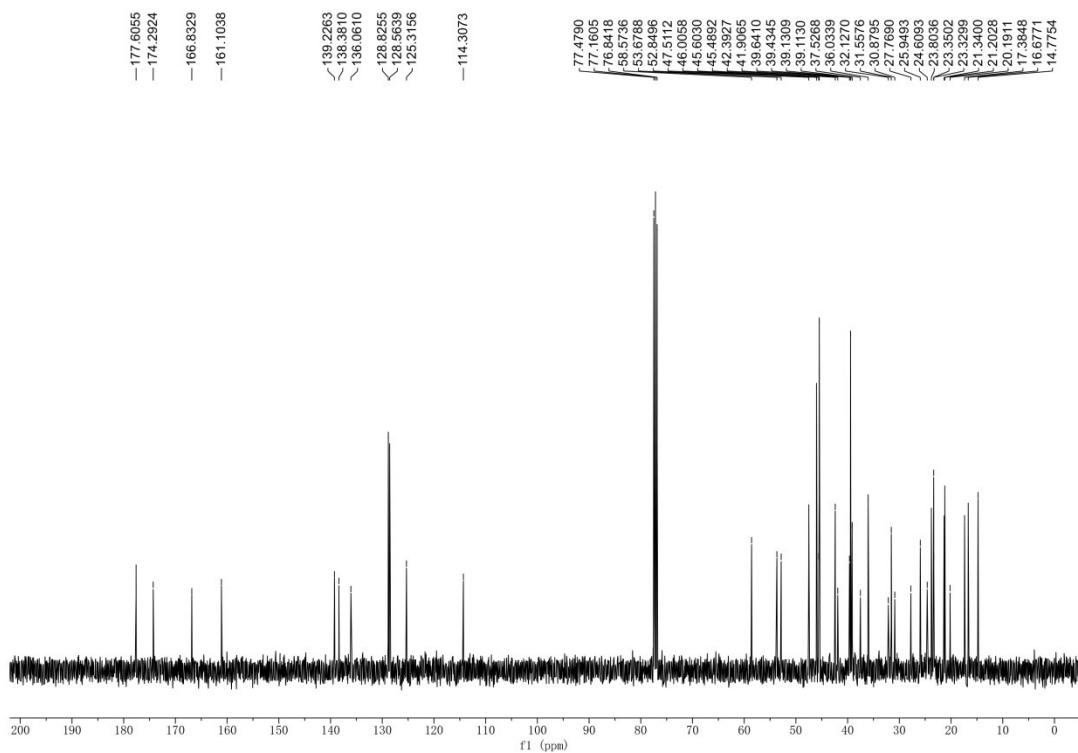


Fig. S35. ^{13}C NMR spectrum of compound 7b (150 MHz, CDCl_3)

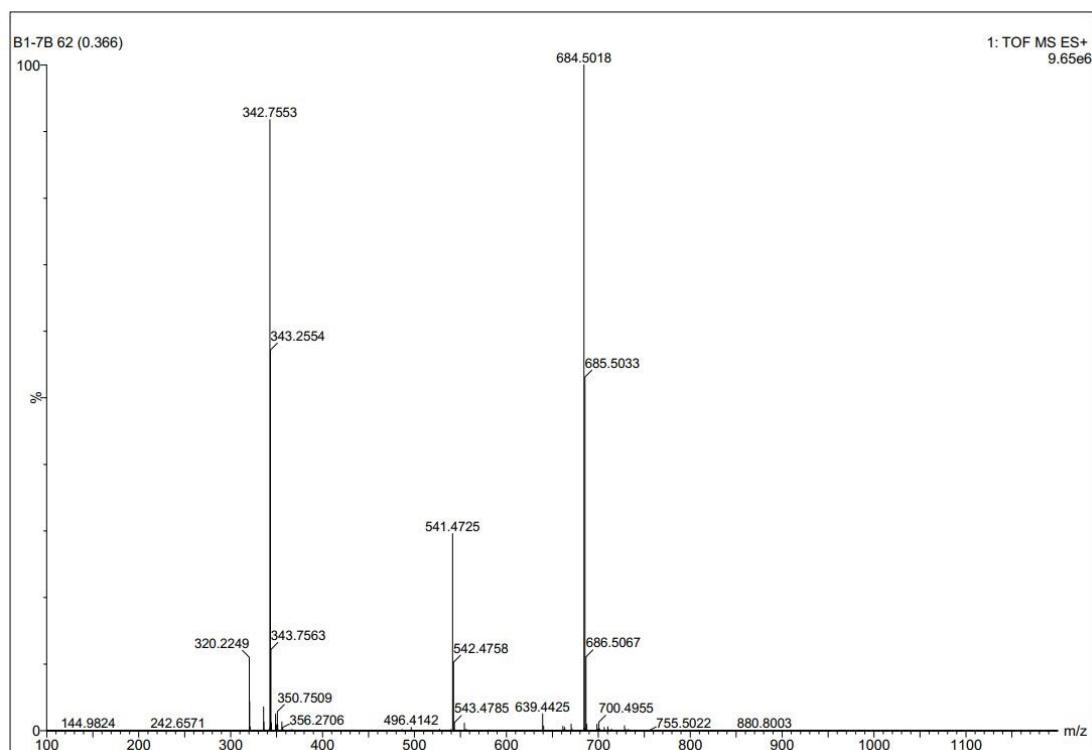


Fig. S36. HRMS spectrum of compound 7b

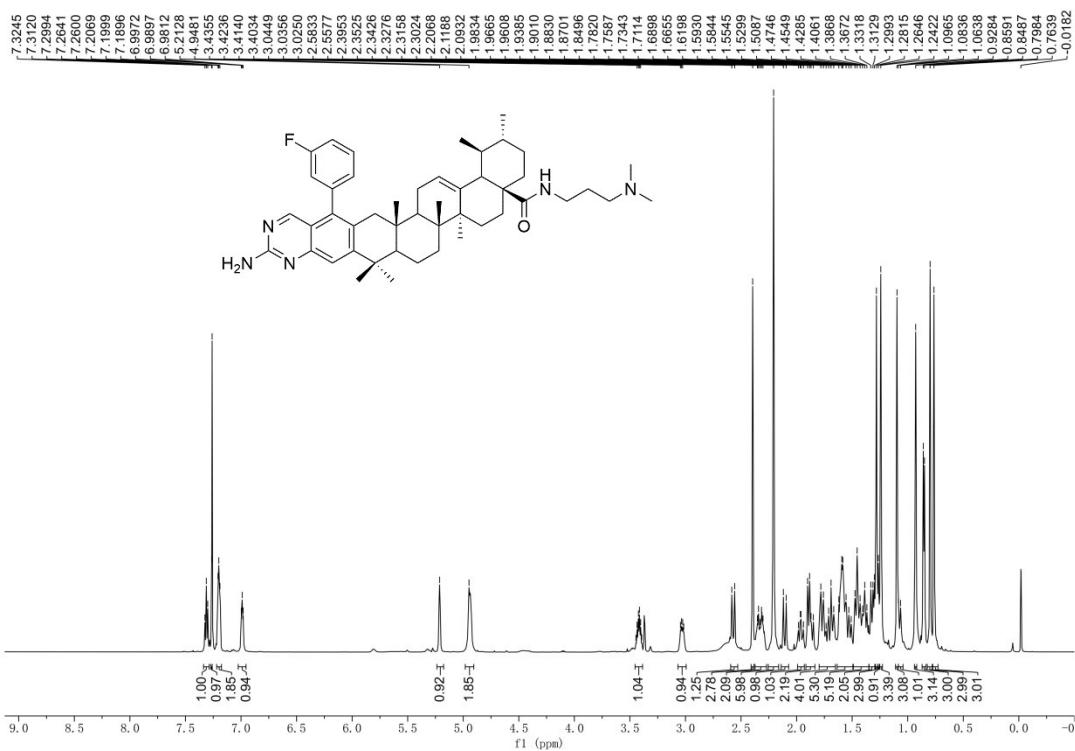


Fig. S37. ¹H NMR spectrum of compound 7c (600 MHz, CDCl₃)

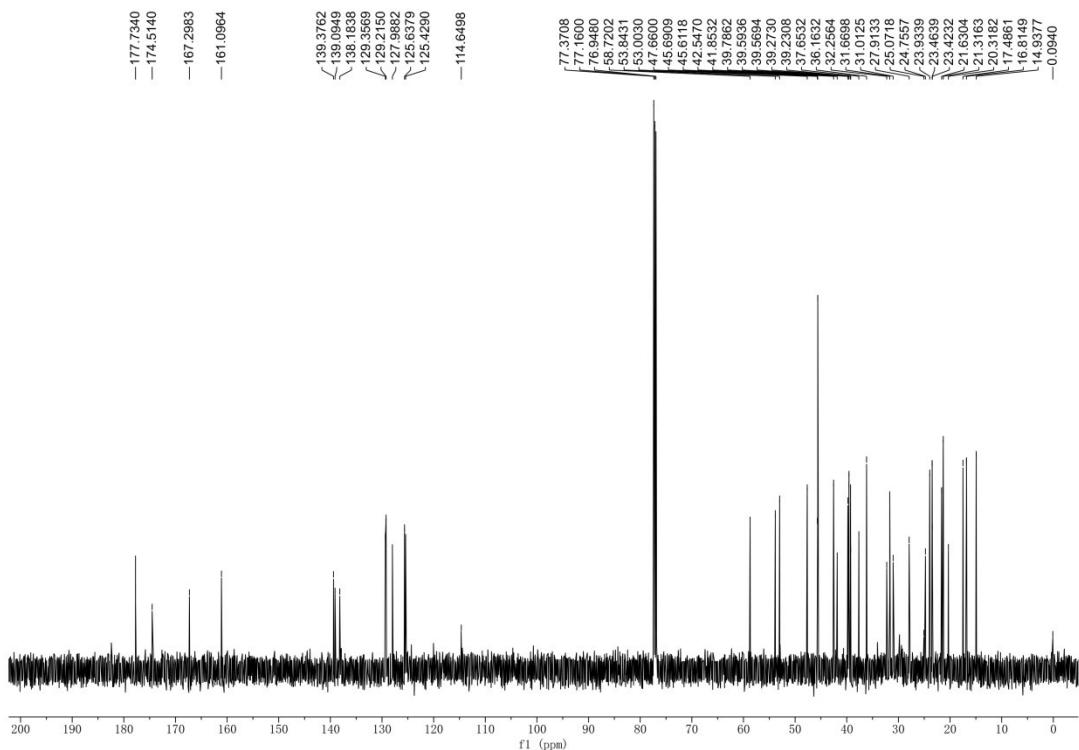


Fig. S38. ¹³C NMR spectrum of compound 7c (150 MHz, CDCl₃)

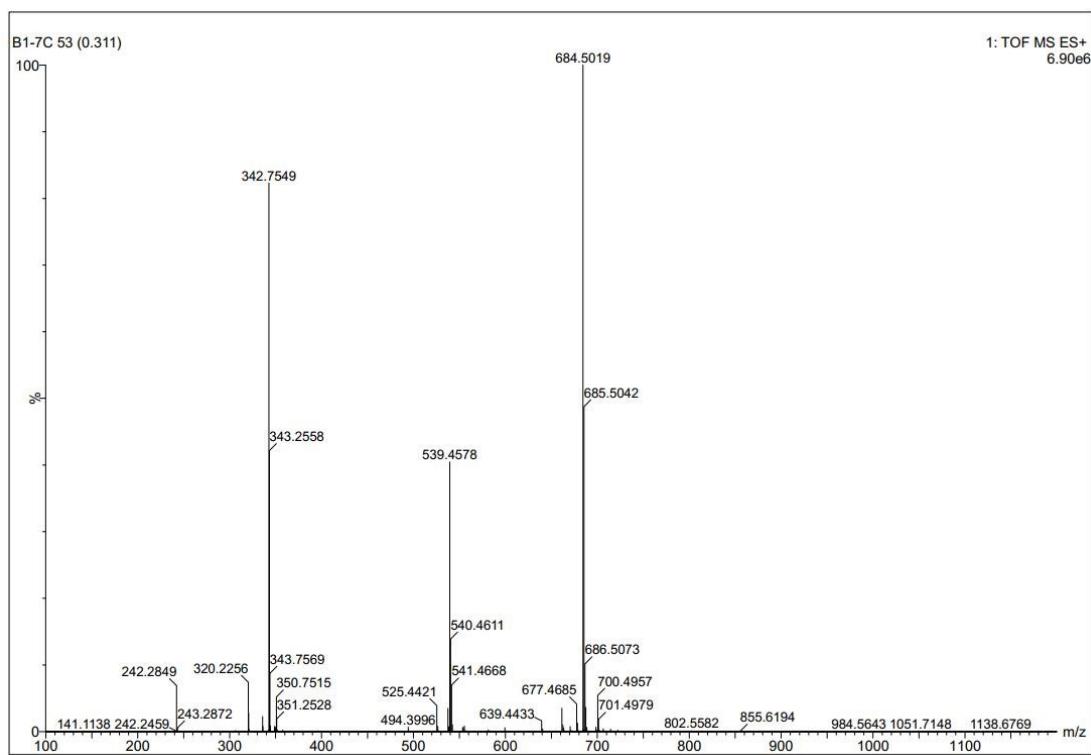


Fig. S39. HRMS spectrum of compound 7c

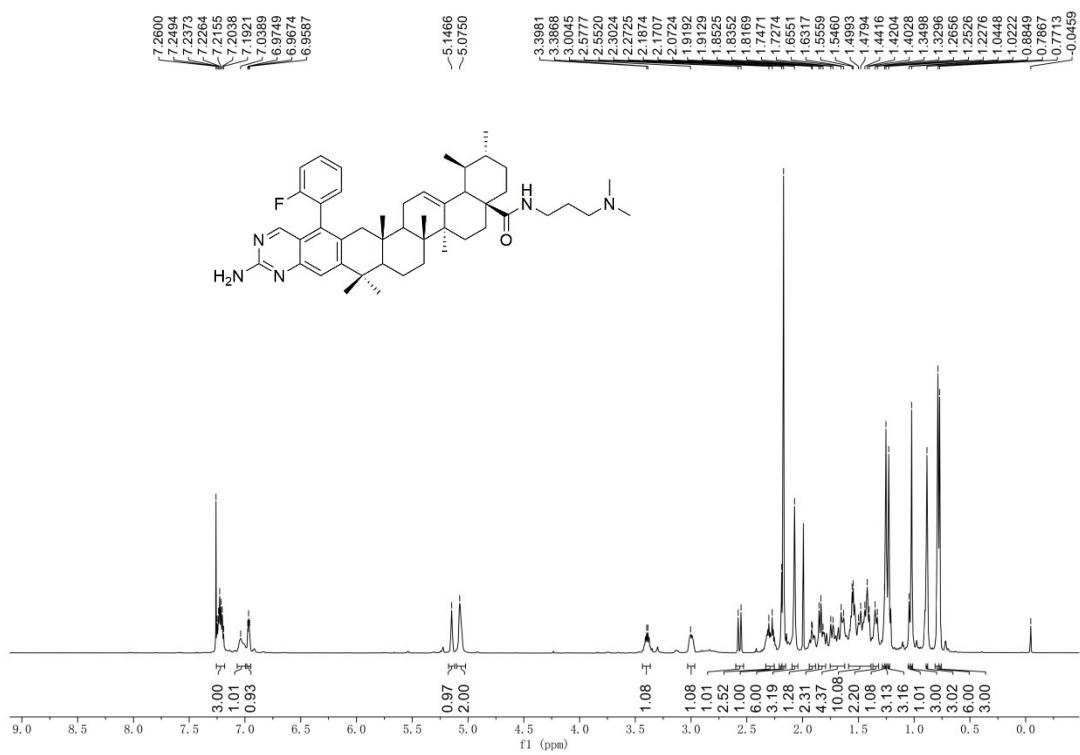


Fig. S40. ¹H NMR spectrum of compound 7d (600 MHz, CDCl₃)

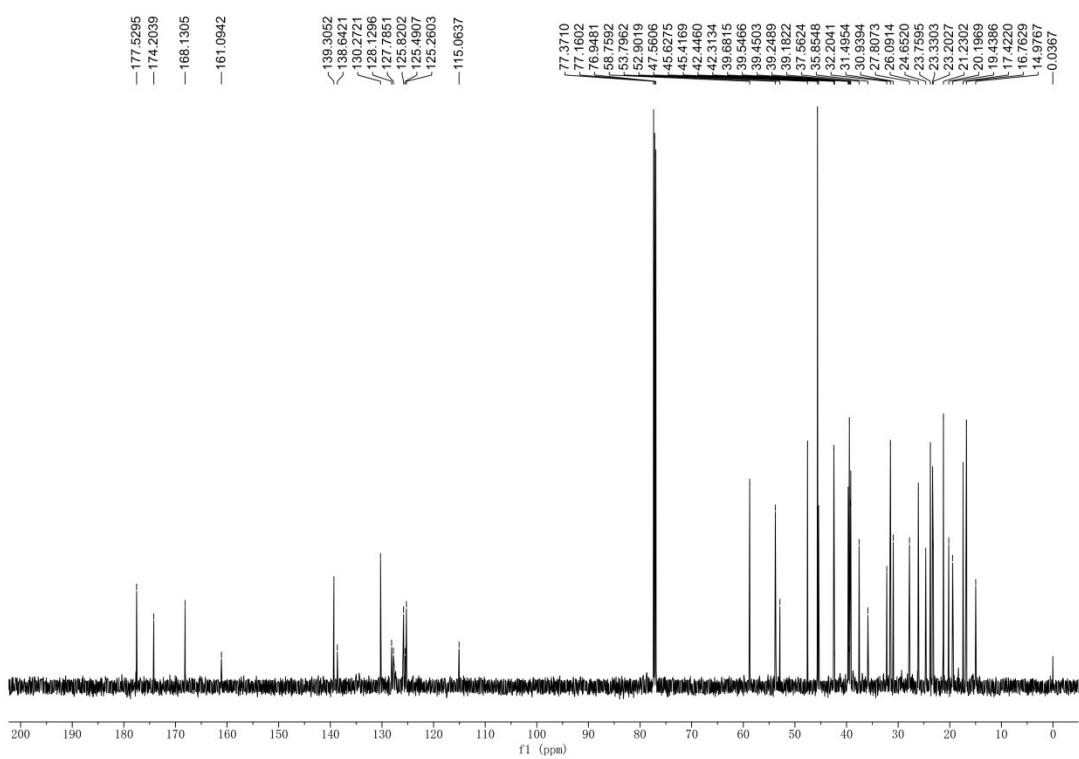


Fig. S41. ¹³C NMR spectrum of compound 7d (150 MHz, CDCl₃)

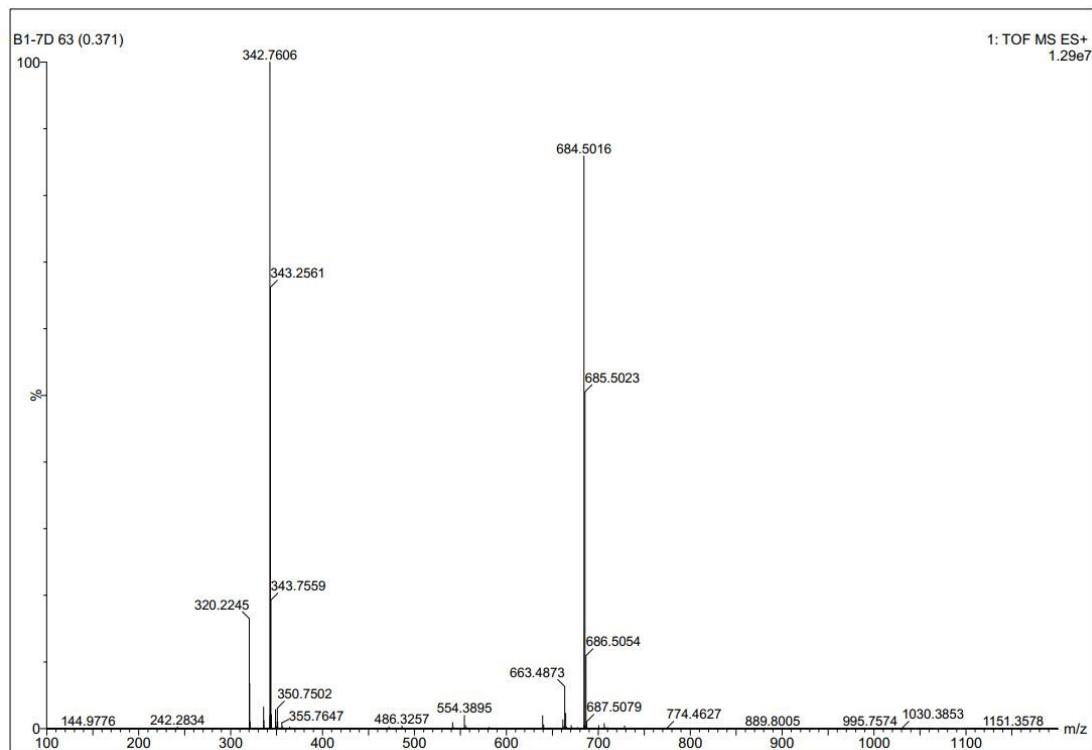


Fig. S42. HRMS spectrum of compound 7d

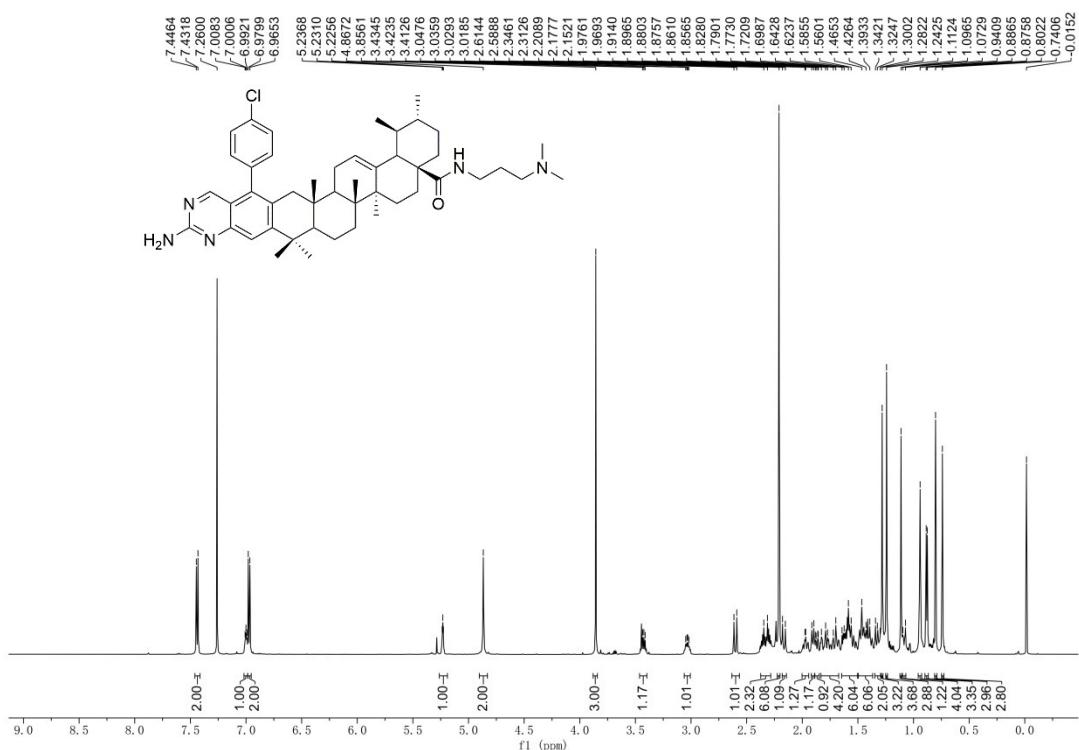


Fig. S43. ¹H NMR spectrum of compound 7e (600 MHz, CDCl₃)

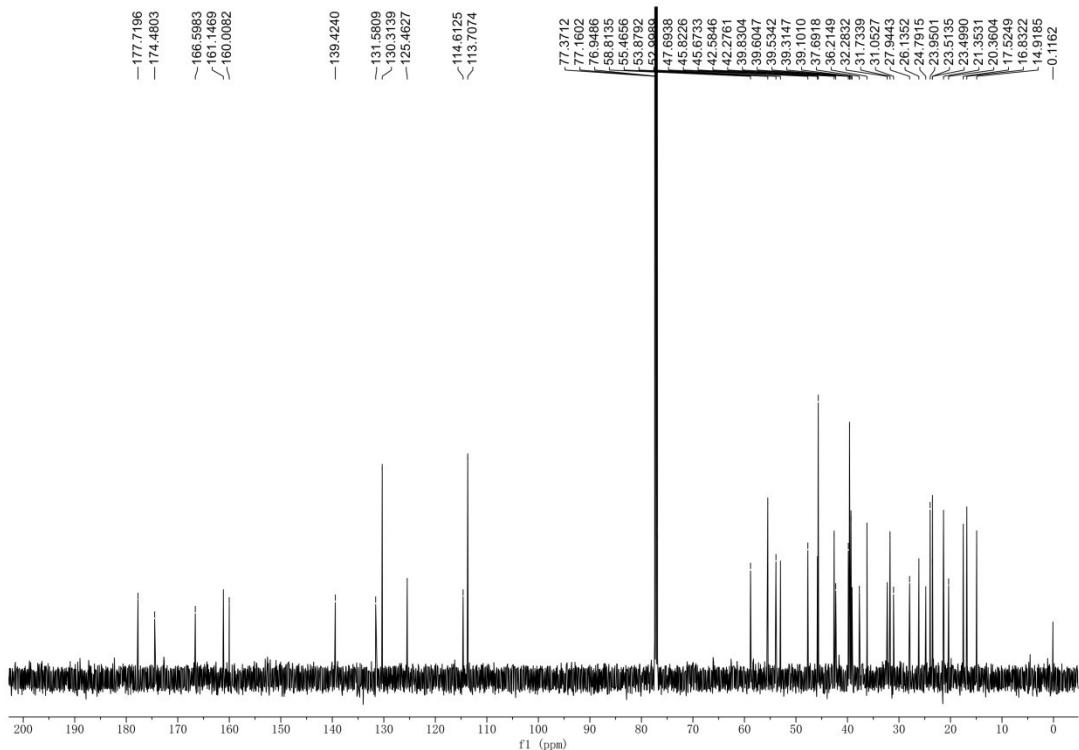


Fig. S44. ¹³C NMR spectrum of compound 7e (150 MHz, CDCl₃)

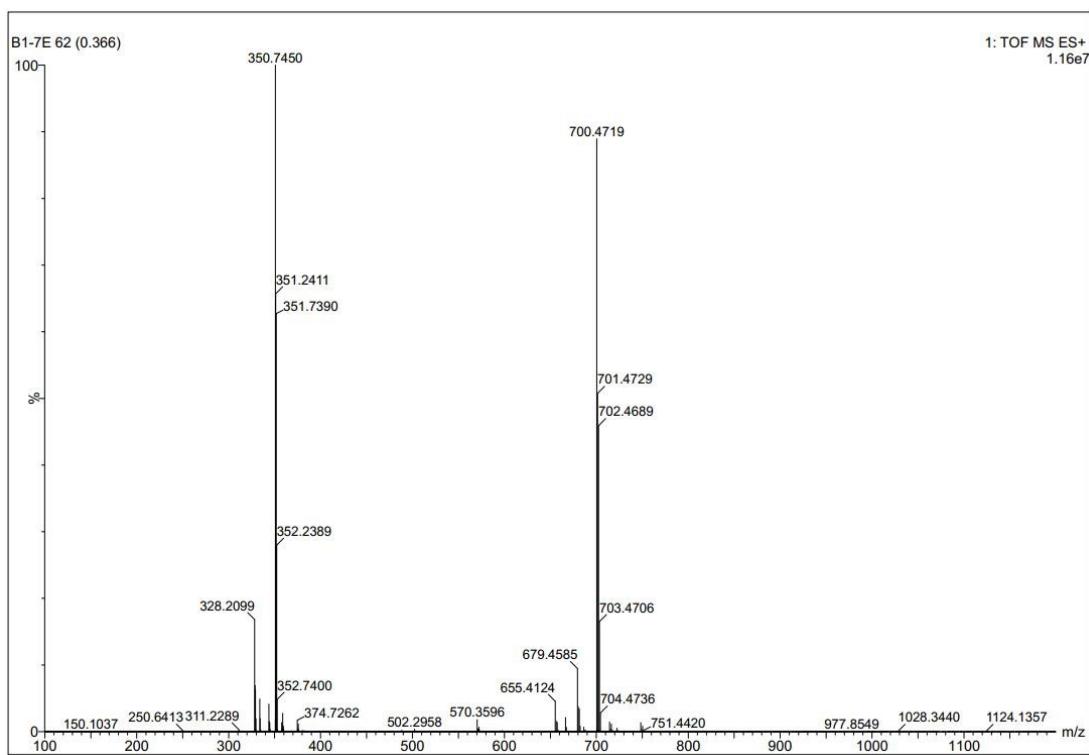


Fig. S45. HRMS spectrum of compound 7e

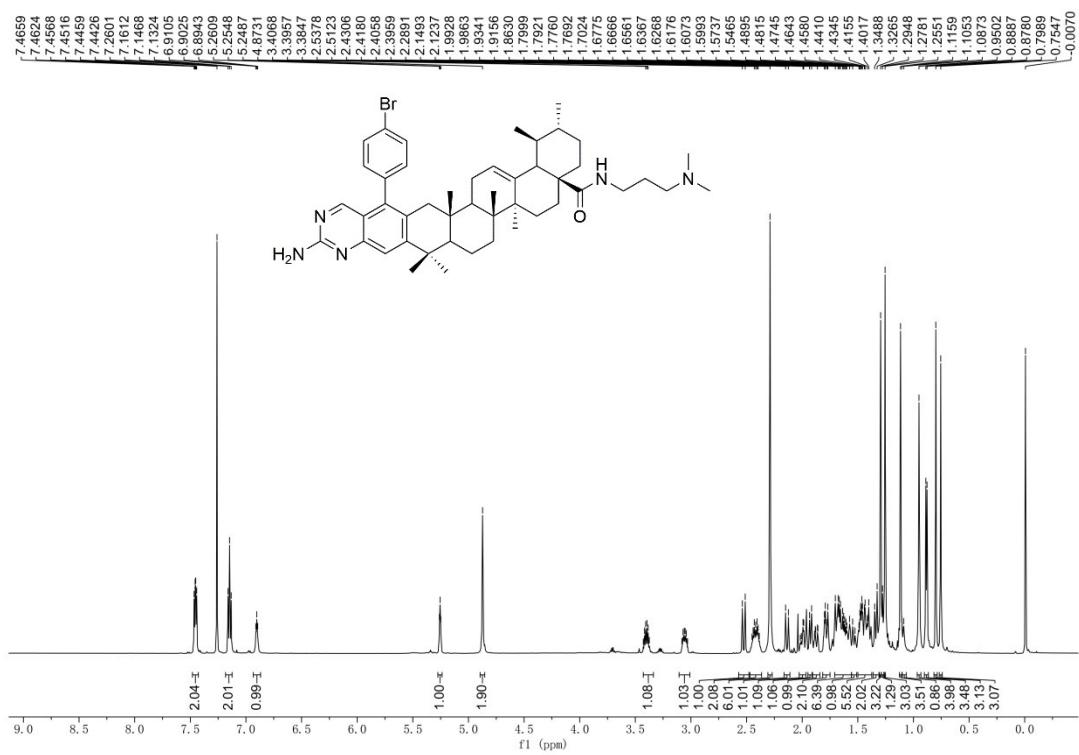


Fig. S46. ¹H NMR spectrum of compound 7f (600 MHz, CDCl₃)

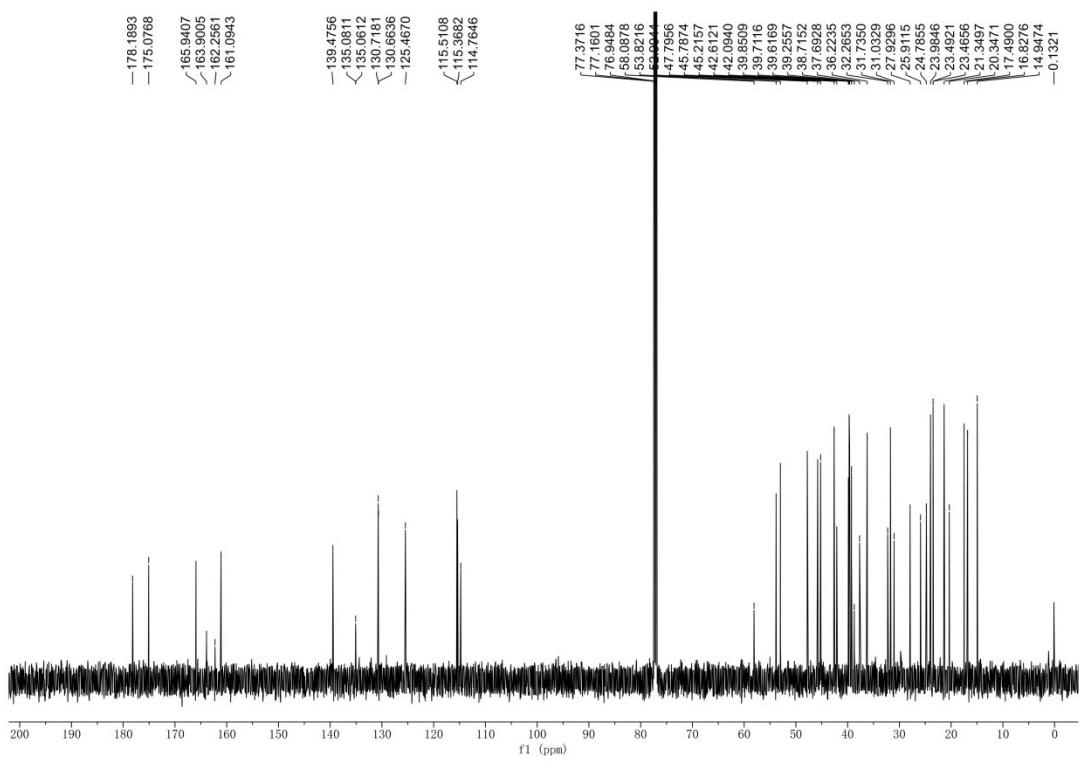


Fig. S47. ^{13}C NMR spectrum of compound 7f (150 MHz, CDCl_3)

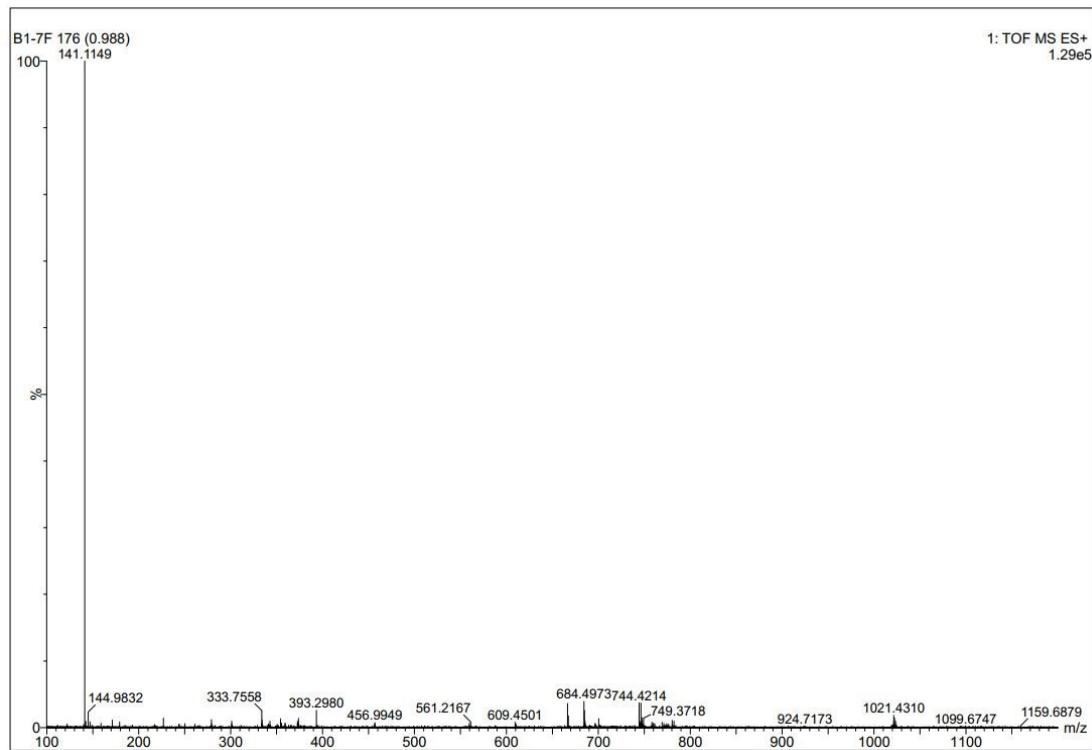


Fig. S48. HRMS spectrum of compound 7f

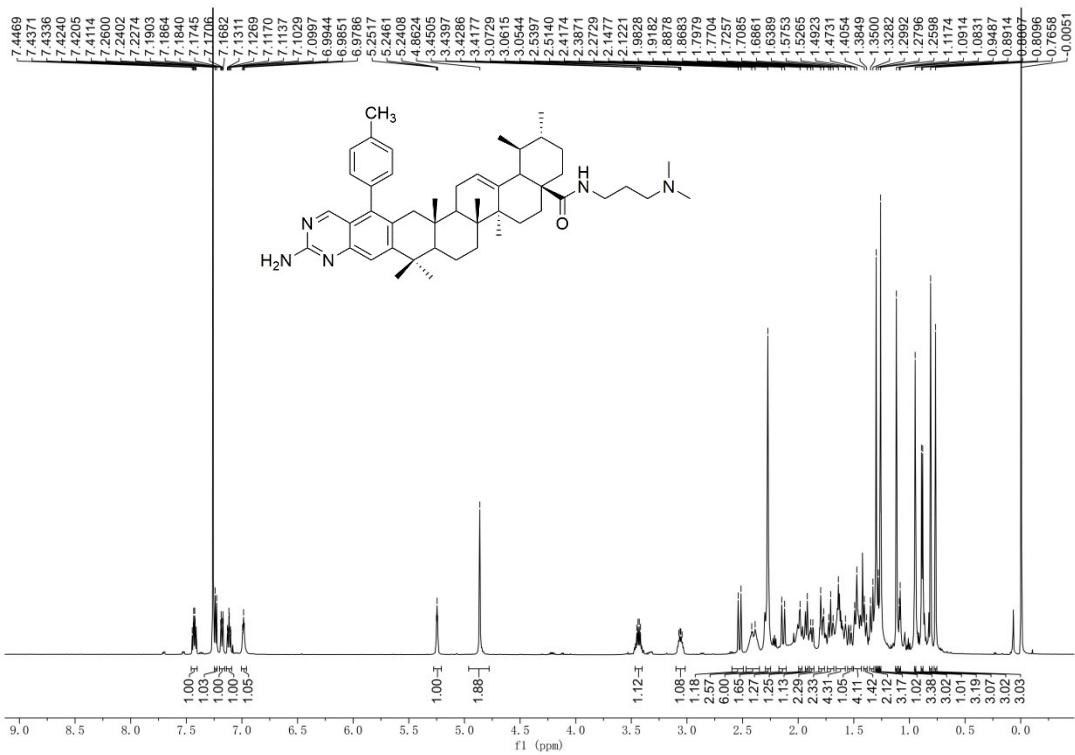


Fig. S49. ^1H NMR spectrum of compound 7g (600 MHz, CDCl_3)

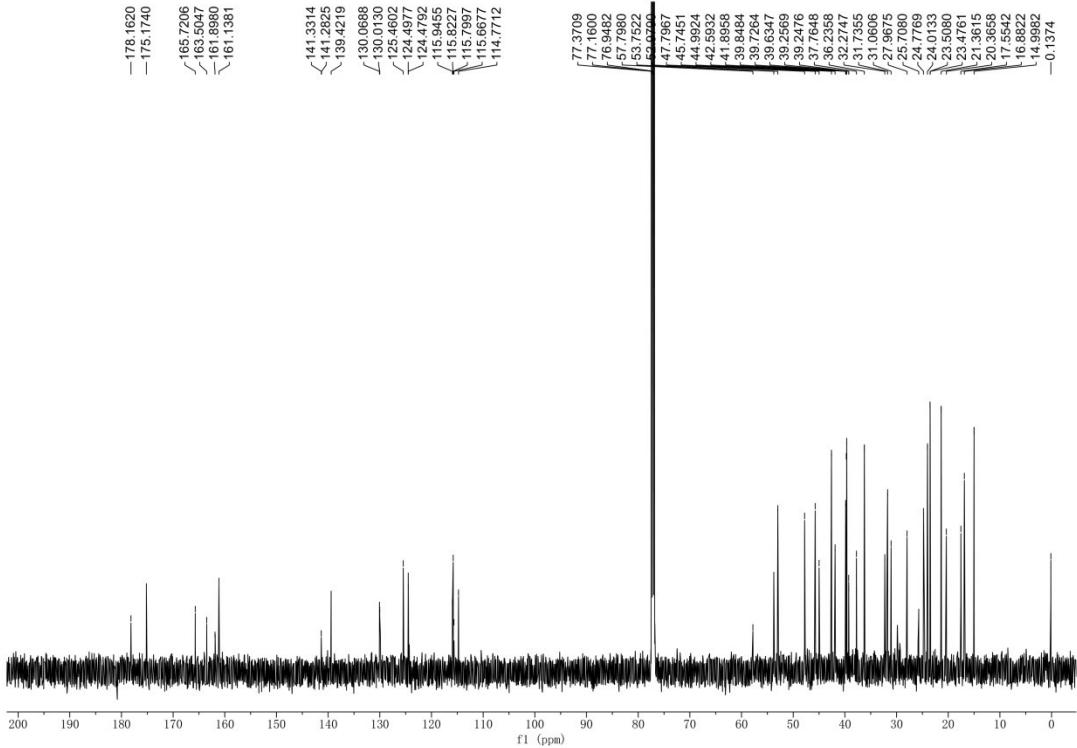


Fig. S50. ^{13}C NMR spectrum of compound 7g (150 MHz, CDCl_3)

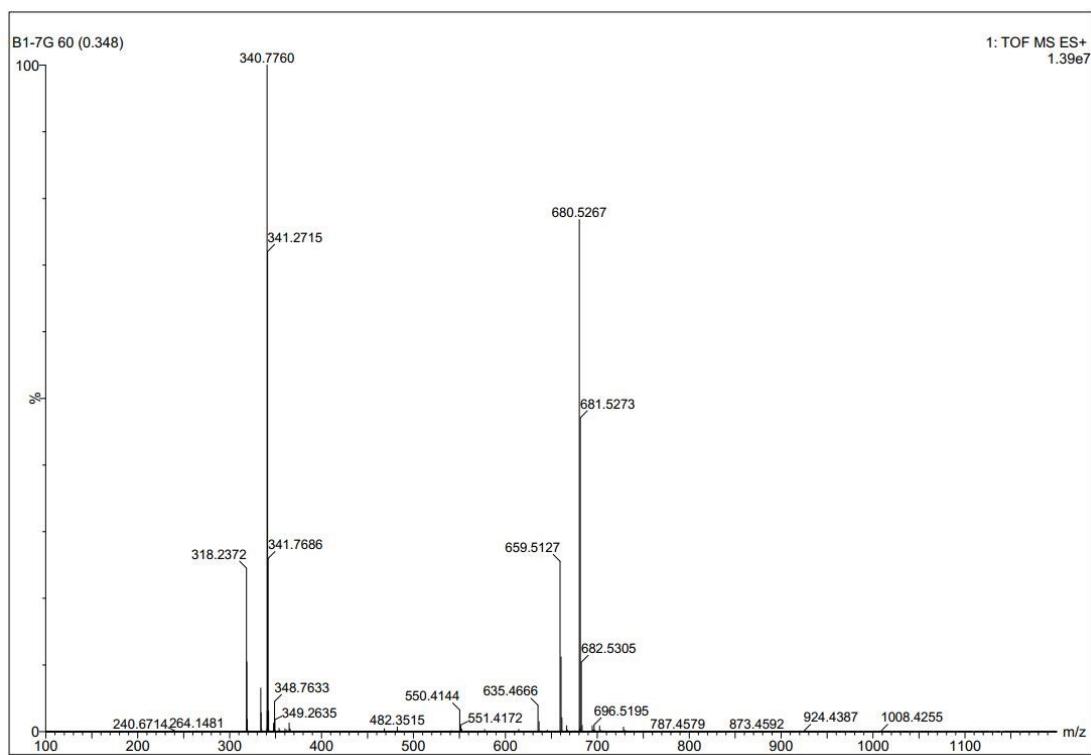


Fig. S51. HRMS spectrum of compound 7g

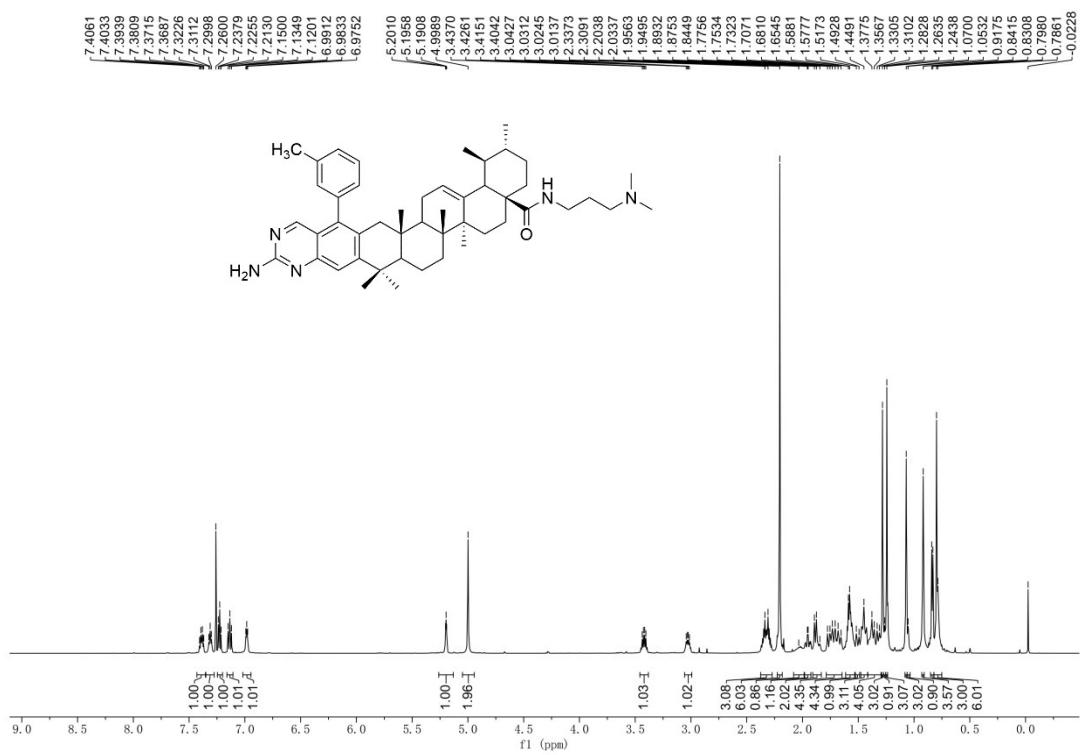


Fig. S52. ¹H NMR spectrum of compound 7h (600 MHz, CDCl₃)

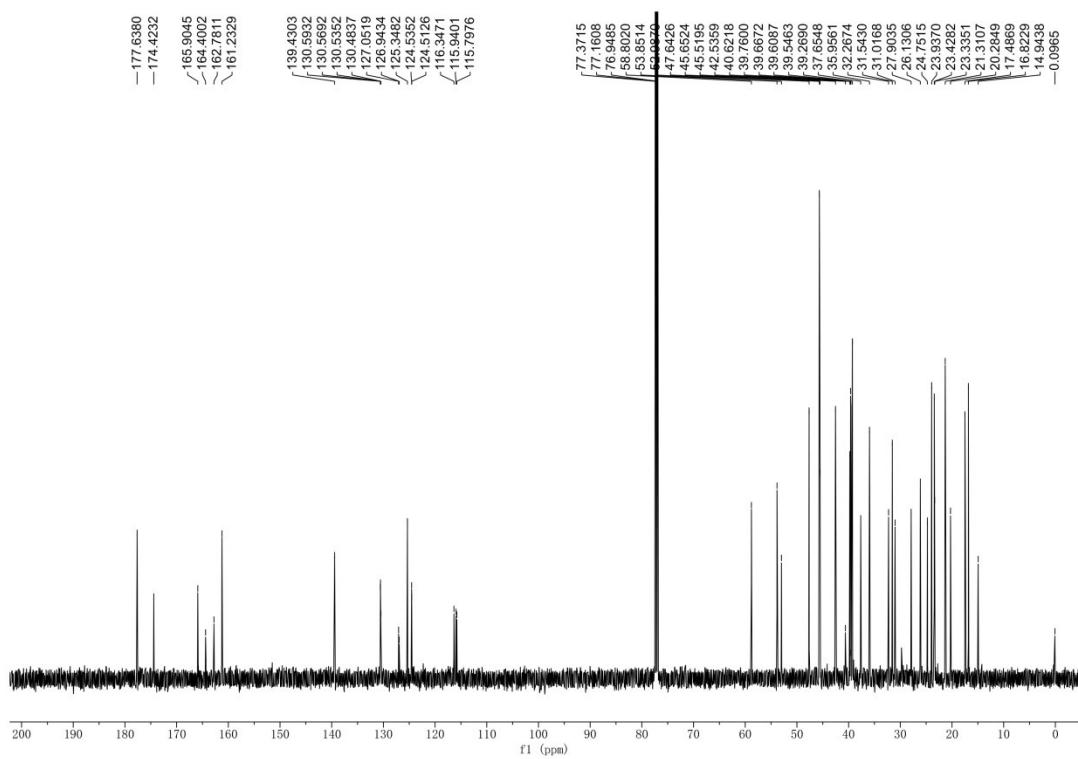


Fig. S53. ^{13}C NMR spectrum of compound 7h (150 MHz, CDCl_3)

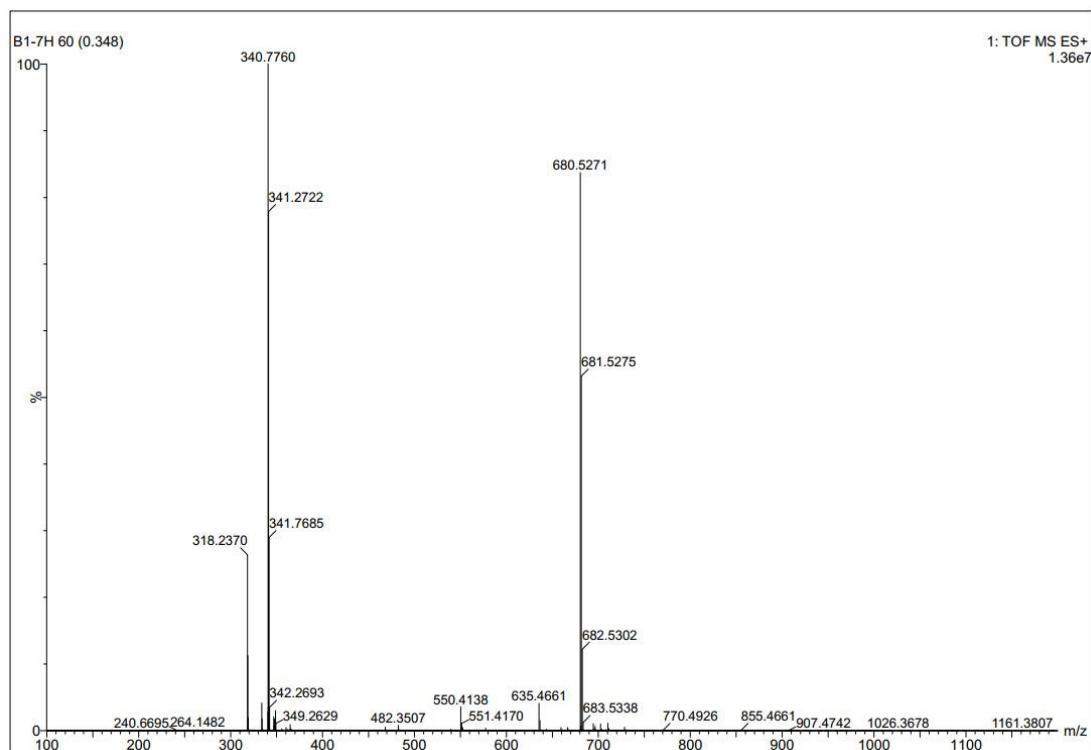


Fig. S54. HRMS spectrum of compound 7h

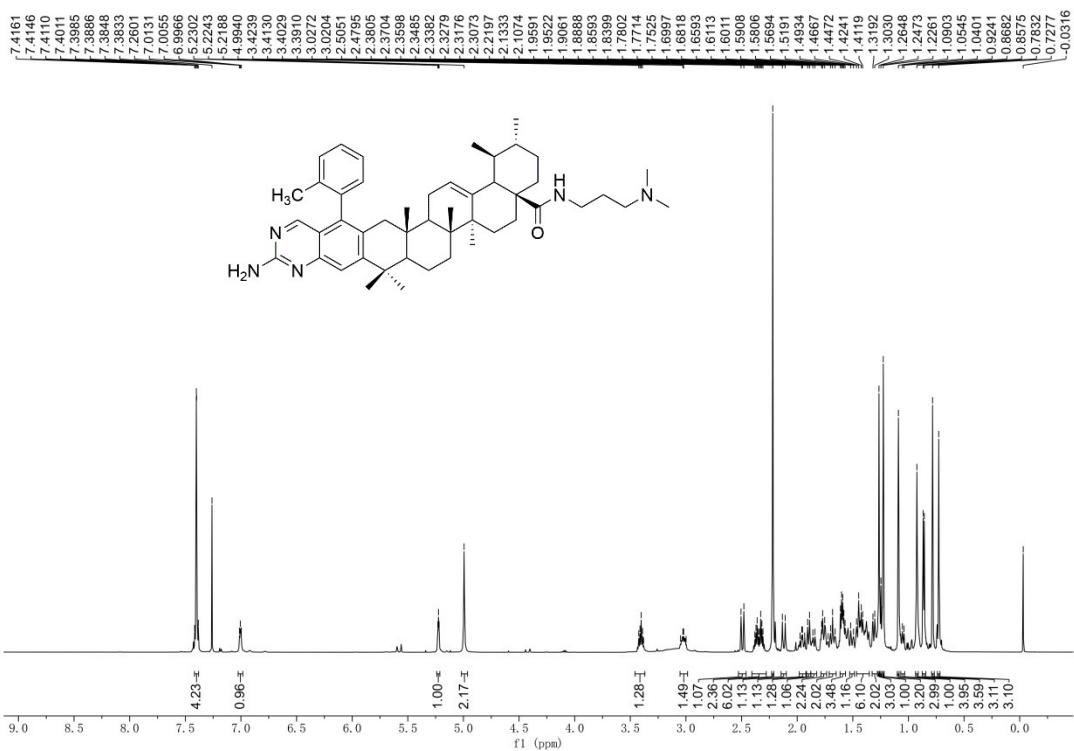


Fig. S55. ^1H NMR spectrum of compound 7i (600 MHz, CDCl_3)

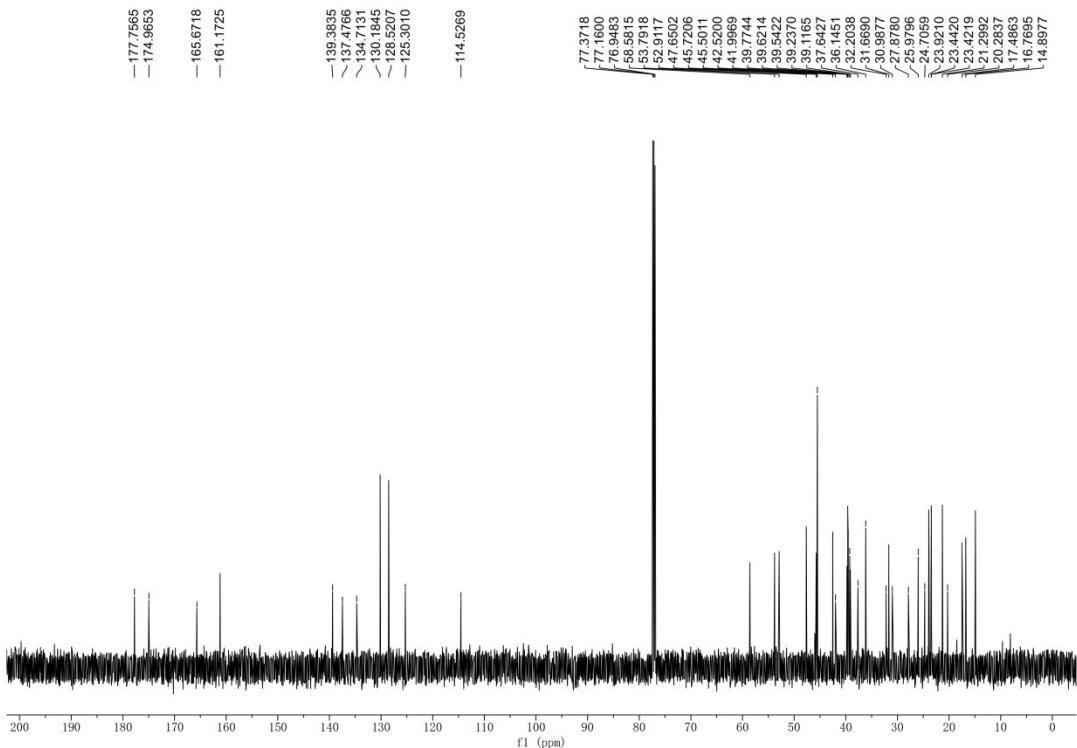


Fig. S56. ^{13}C NMR spectrum of compound 7i (150 MHz, CDCl_3)

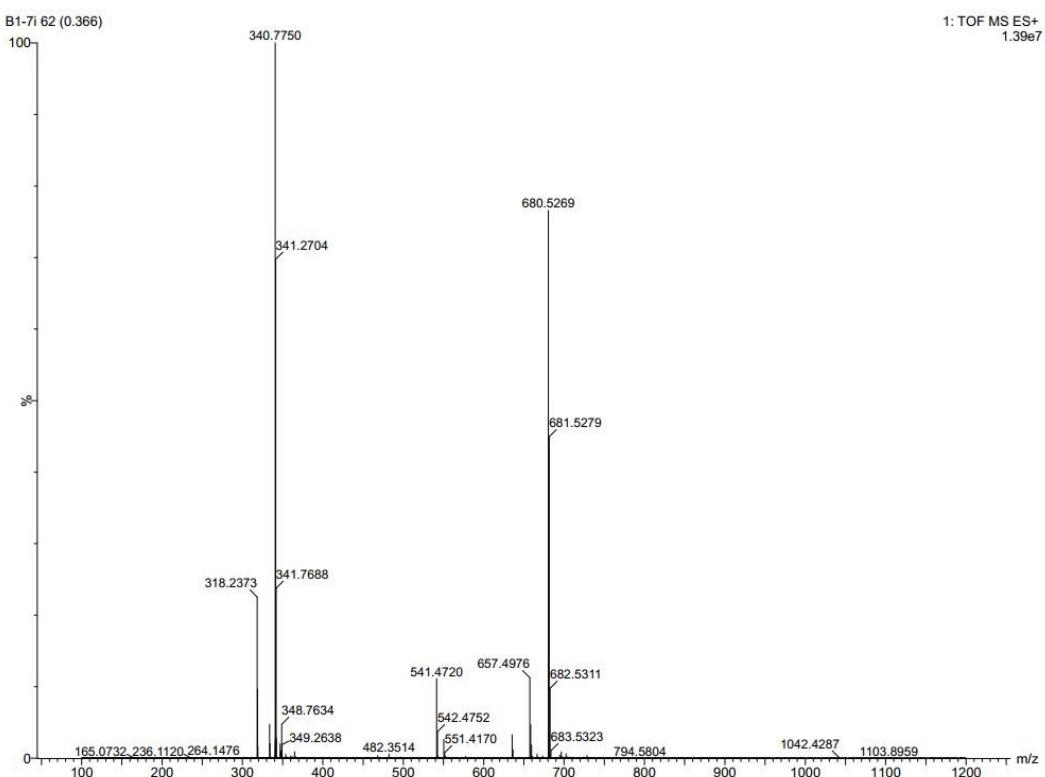


Fig. S57. HRMS spectrum of compound 7i

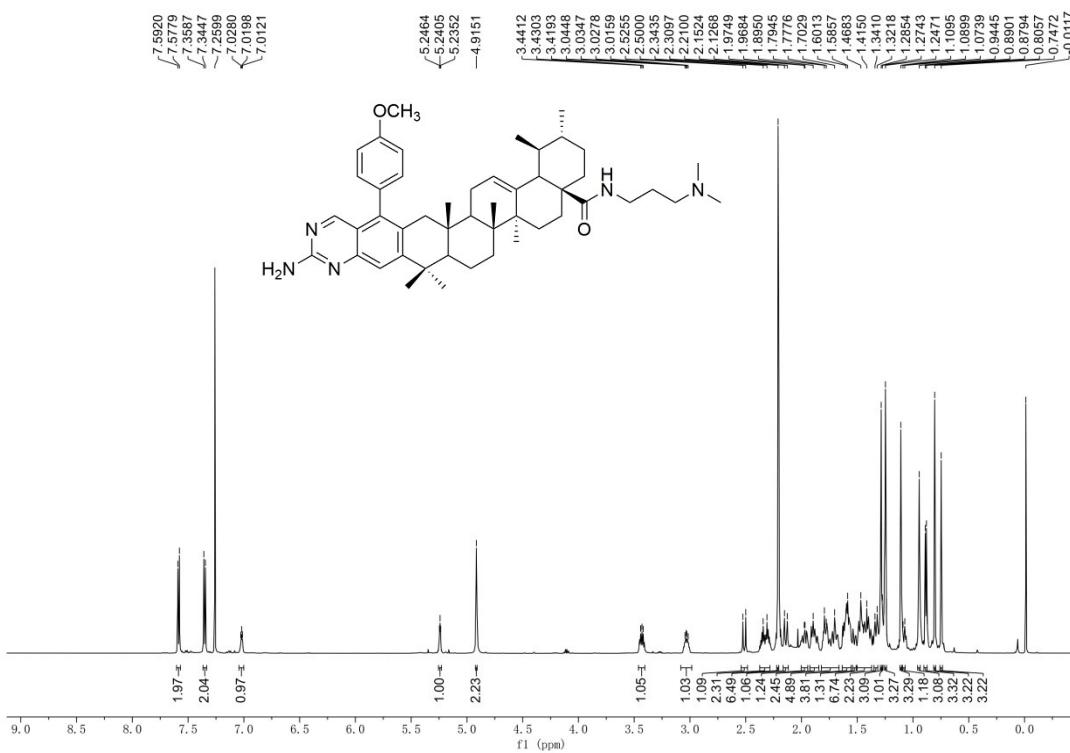


Fig. S58. ^1H NMR spectrum of compound 7j (600 MHz, CDCl_3)

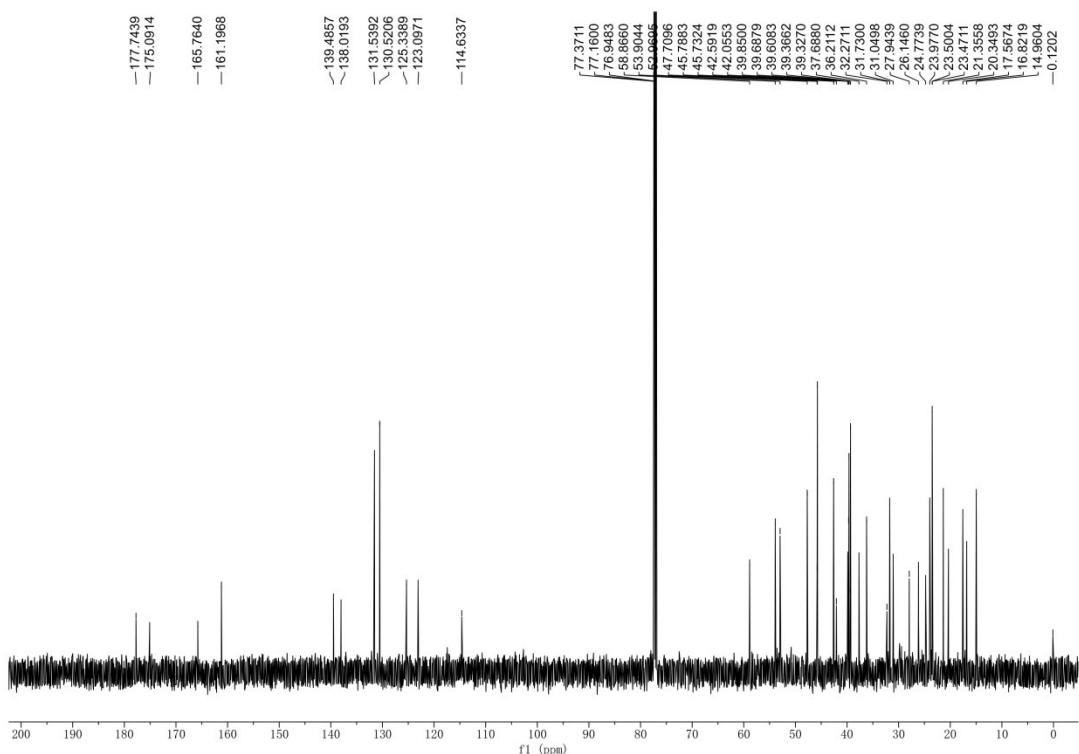


Fig. S59. ^{13}C NMR spectrum of compound 7j (150 MHz, CDCl_3)

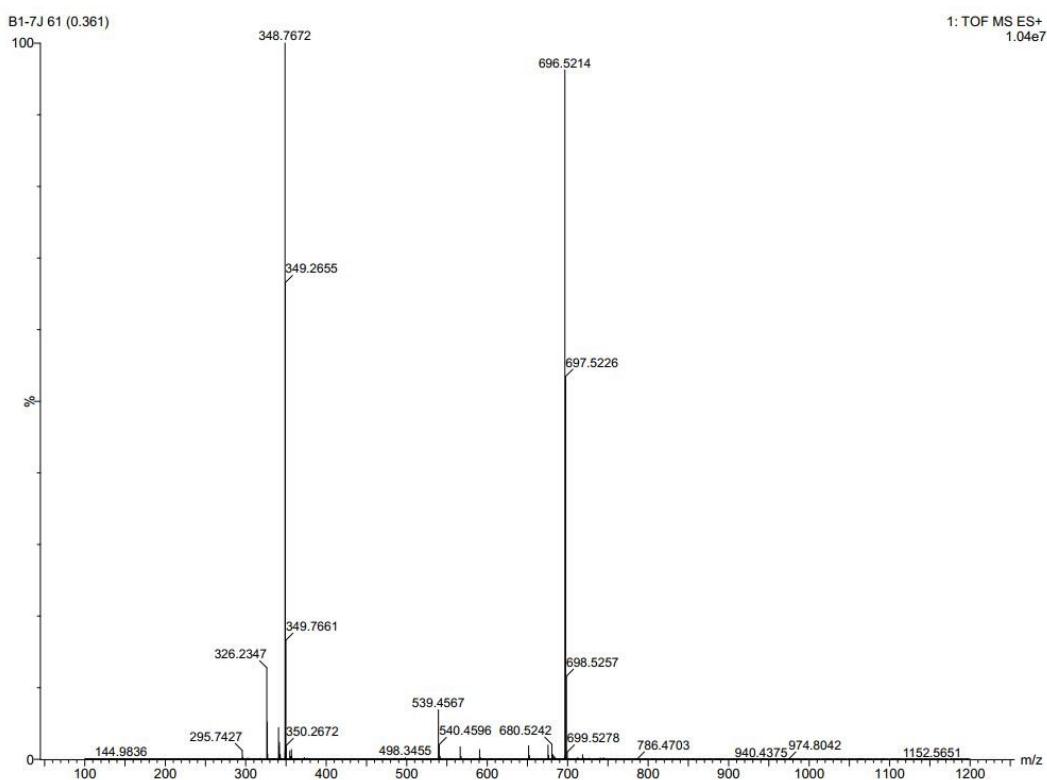


Fig. S60. HRMS spectrum of compound 7j

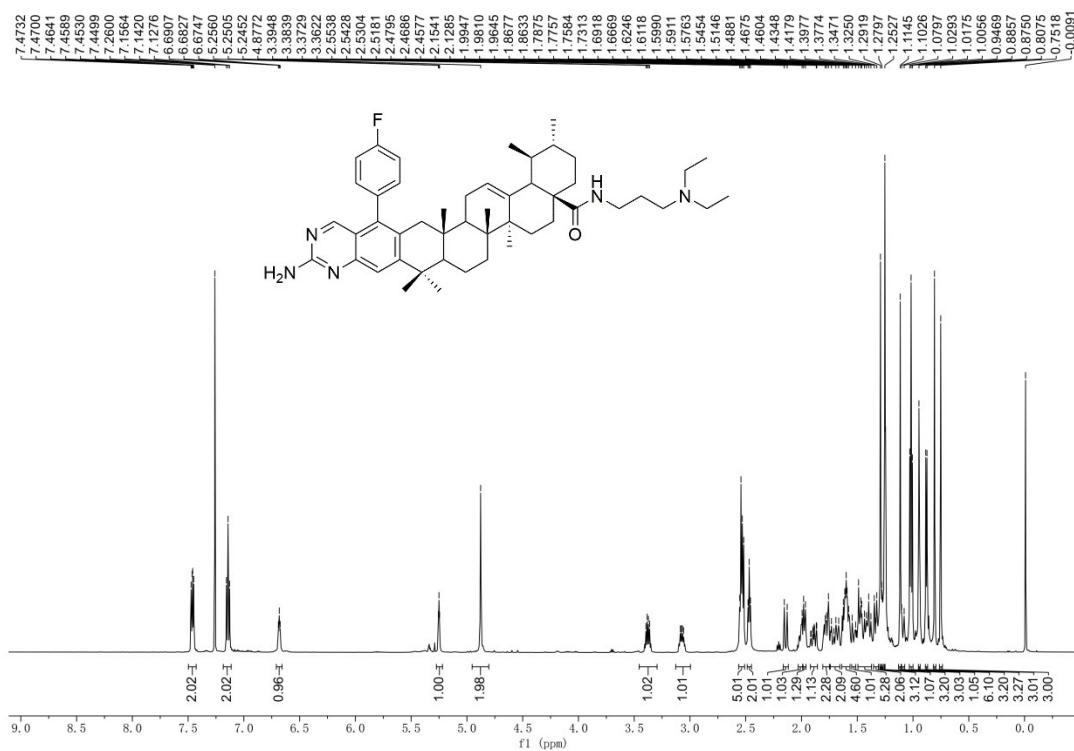


Fig. S61. ^1H NMR spectrum of compound 9a (600 MHz, CDCl_3)

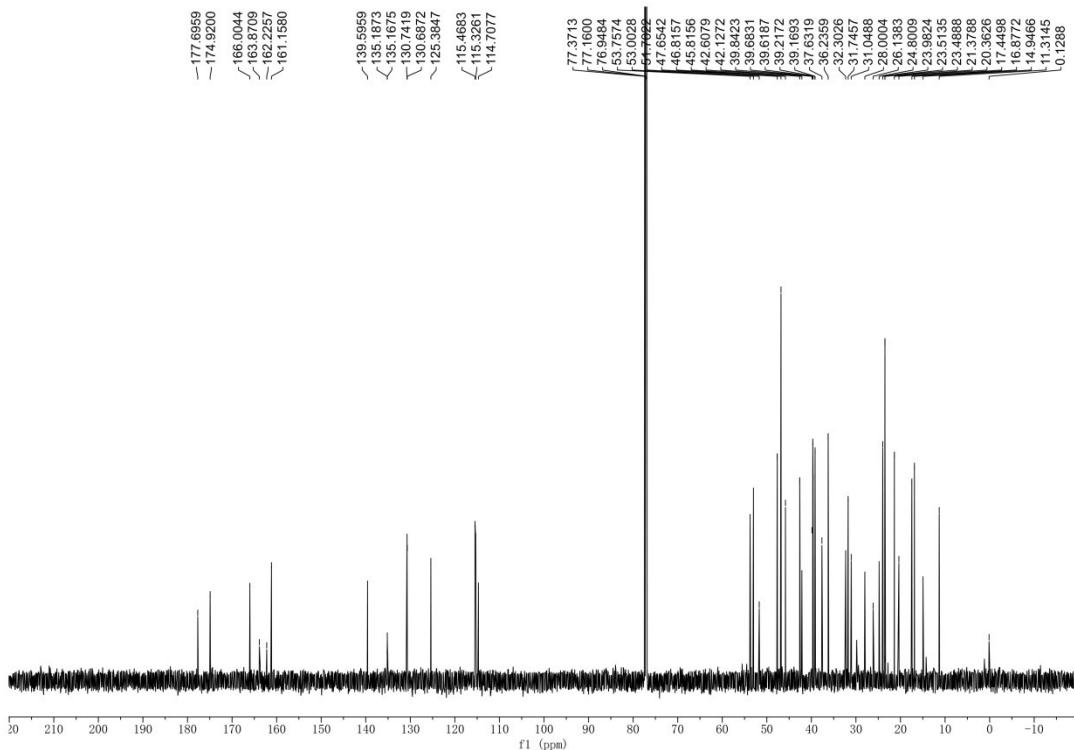


Fig. S62. ^{13}C NMR spectrum of compound 9a (150 MHz, CDCl_3)

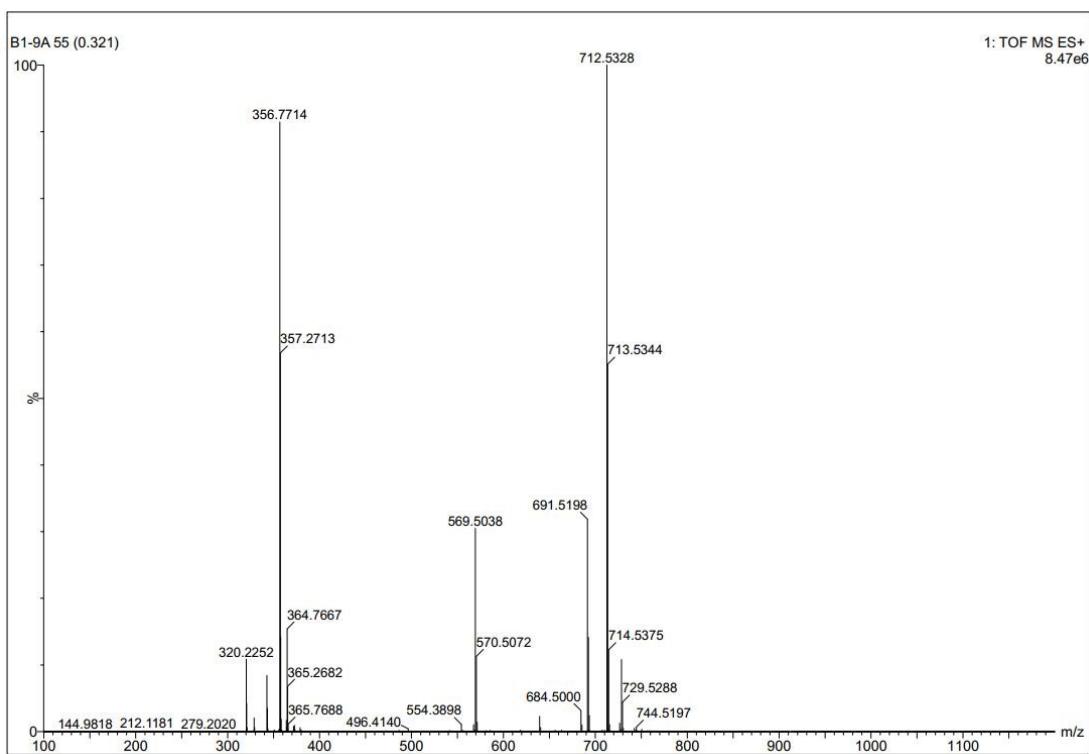


Fig. S63. HRMS spectrum of compound 9a

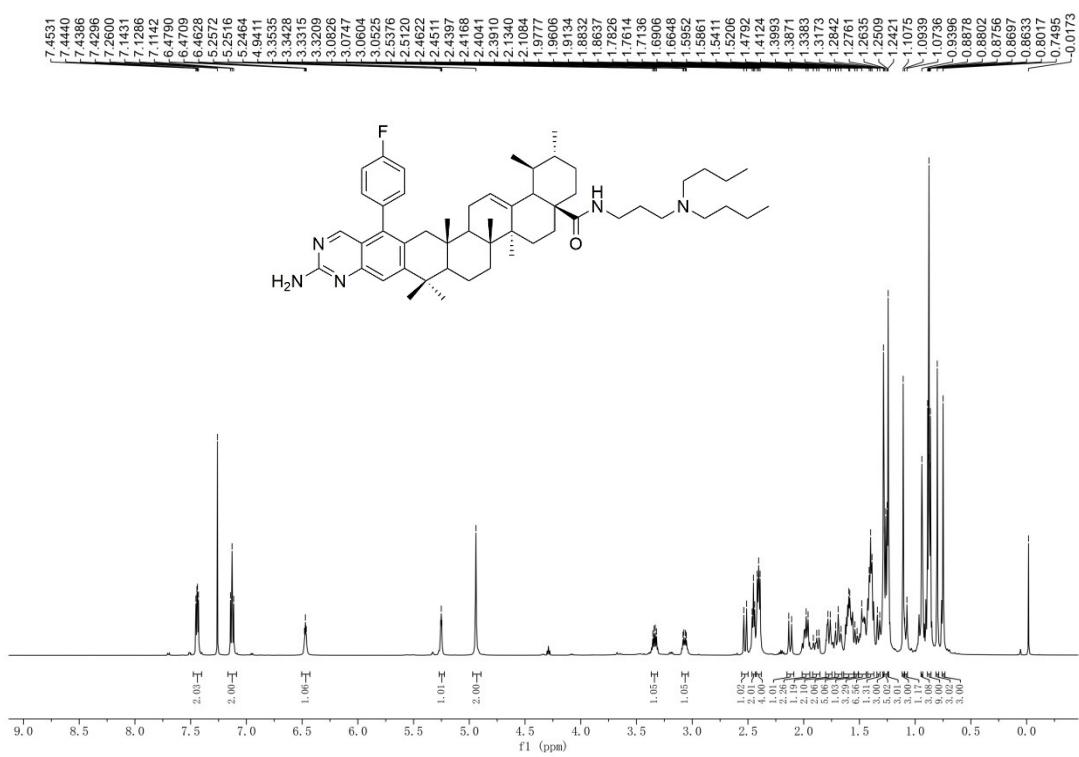


Fig. S64. ^1H NMR spectrum of compound 9b (600 MHz, CDCl_3)

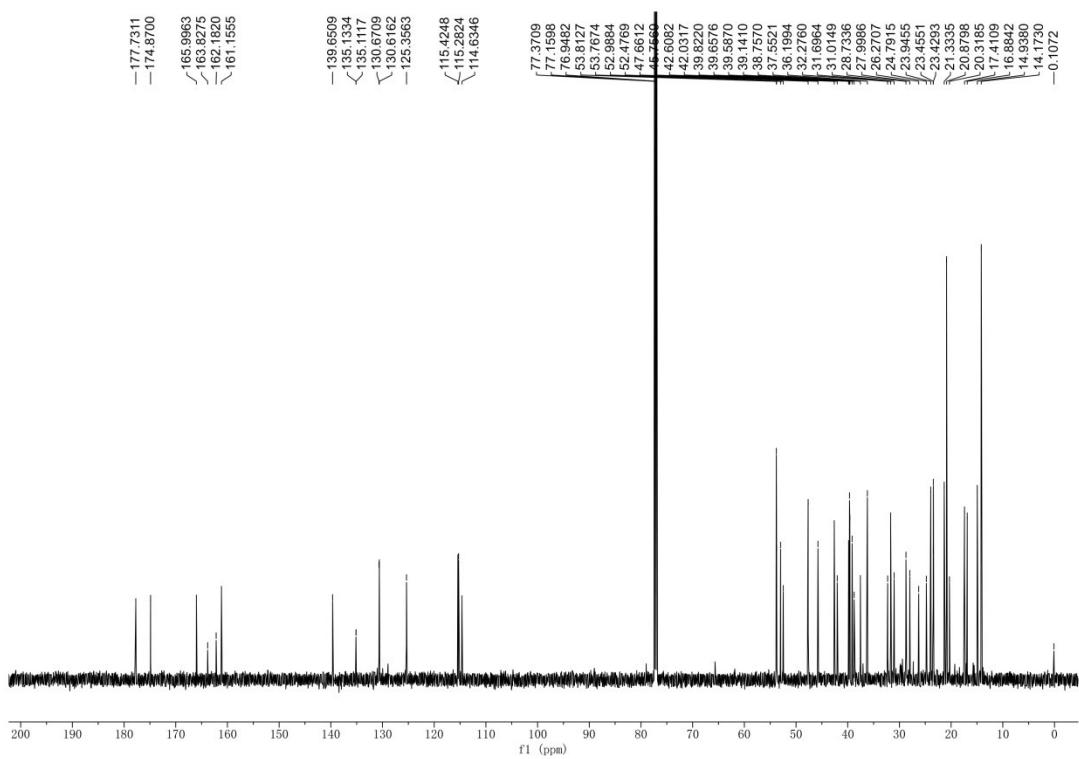


Fig. S65. ^{13}C NMR spectrum of compound 9b (150 MHz, CDCl_3)

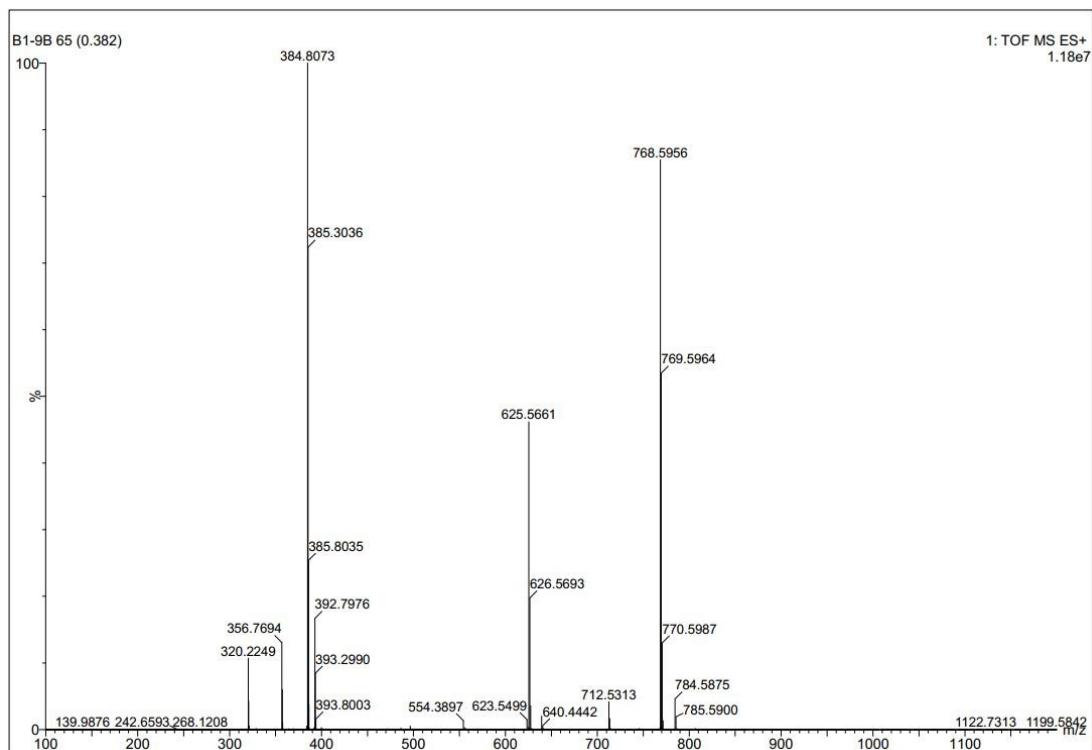


Fig. S66. HRMS spectrum of compound 9b

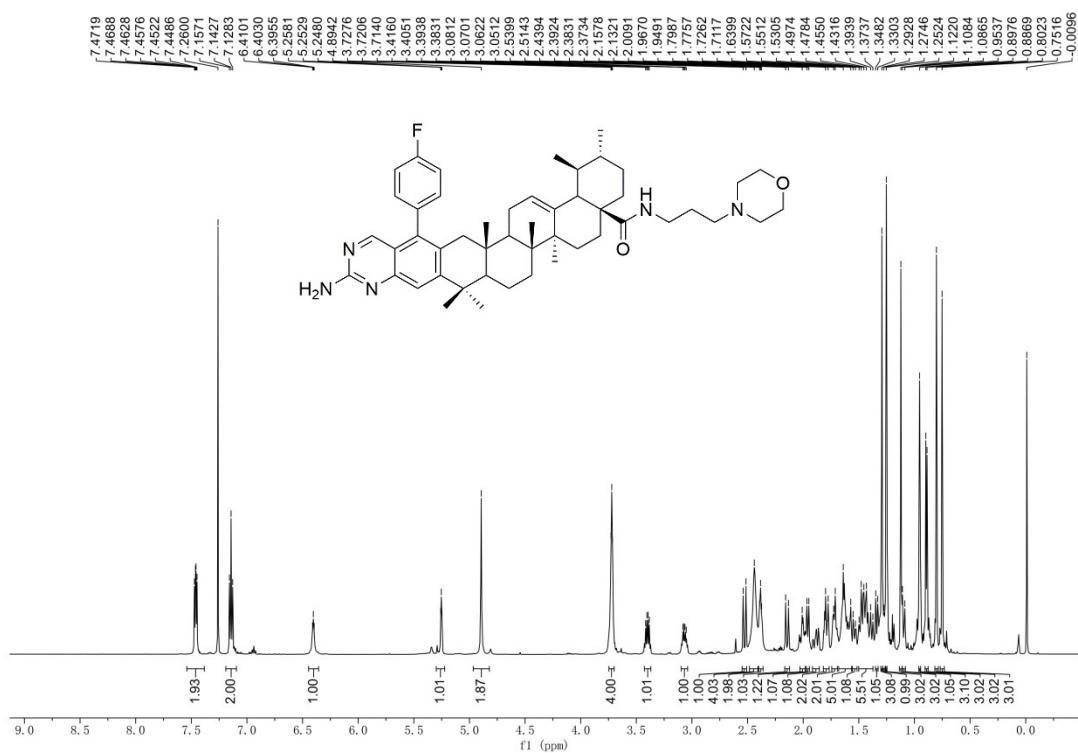


Fig. S67. ^1H NMR spectrum of compound 9c (600 MHz, CDCl_3)

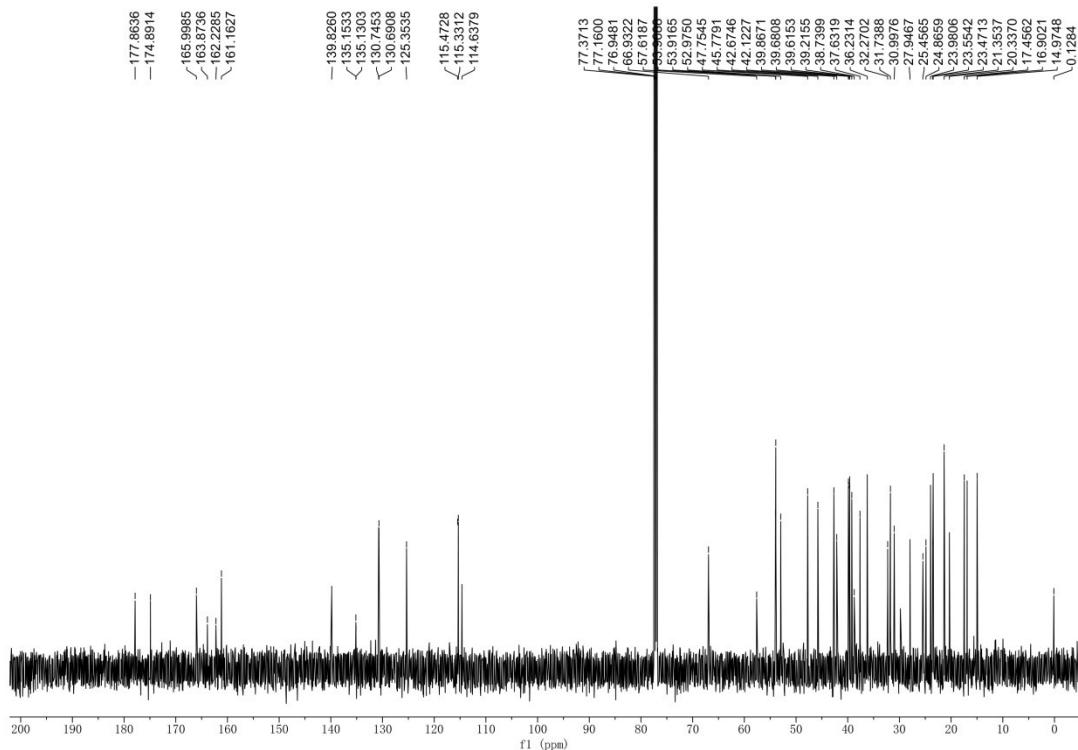


Fig. S68. ^{13}C NMR spectrum of compound 9c (150 MHz, CDCl_3)

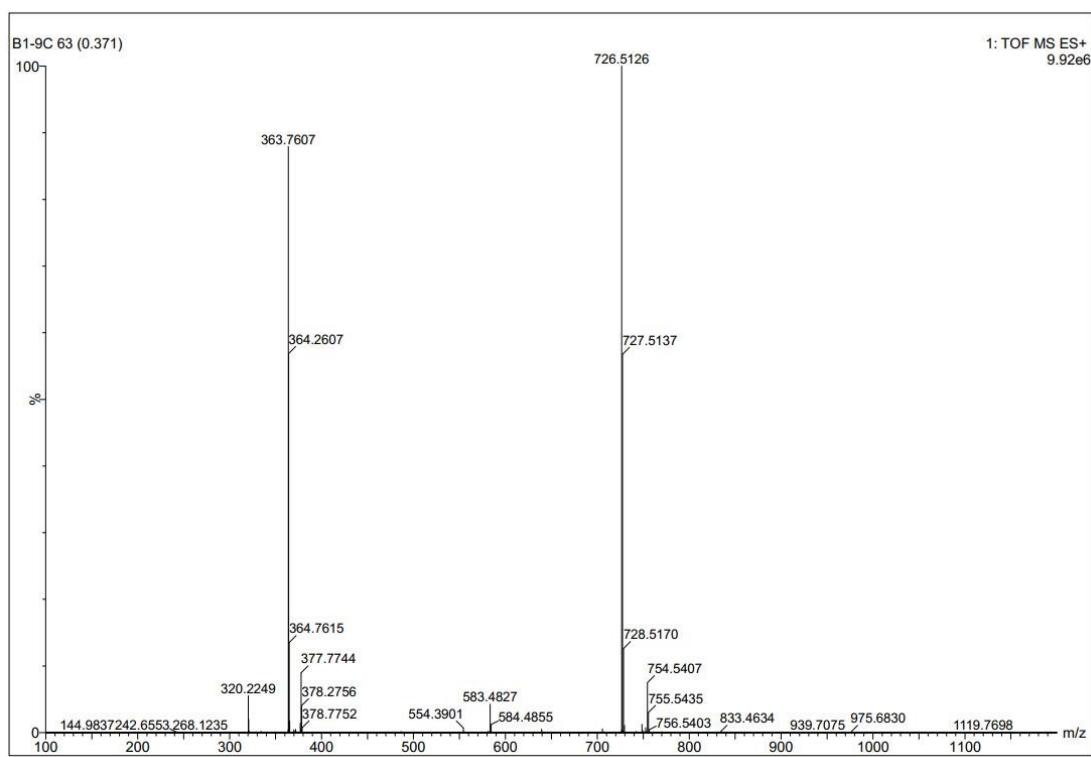


Fig. S69. HRMS spectrum of compound 9c

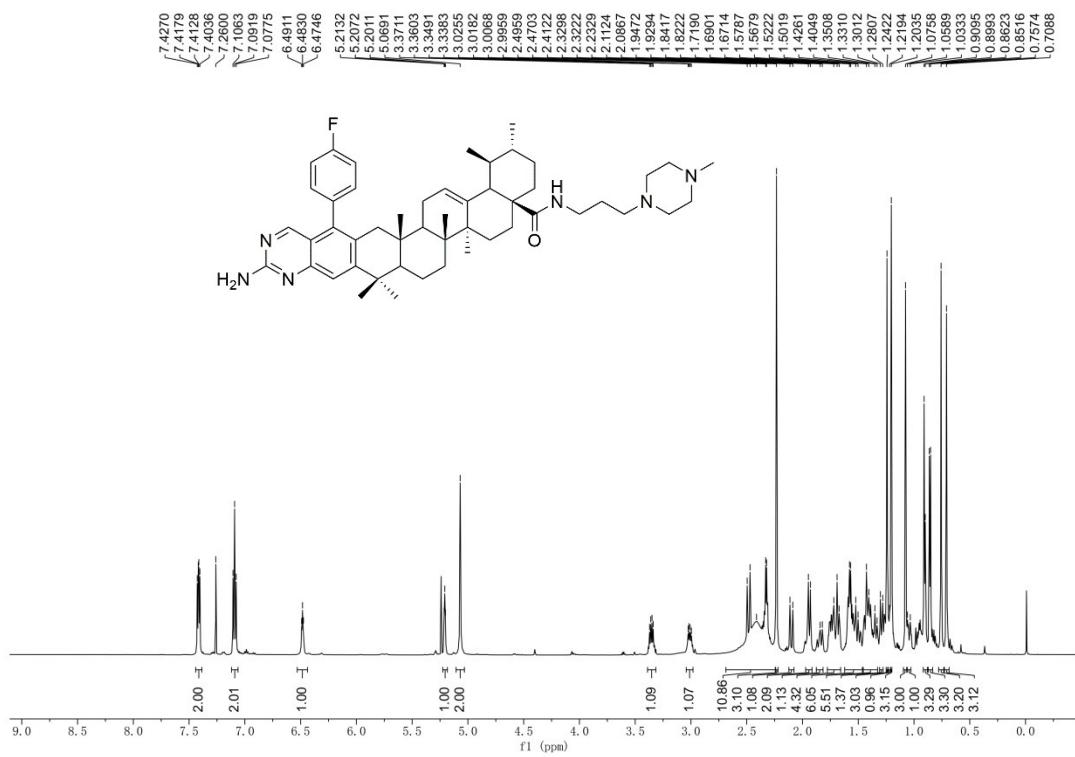


Fig. S70. ¹H NMR spectrum of compound 9d (600 MHz, CDCl₃)

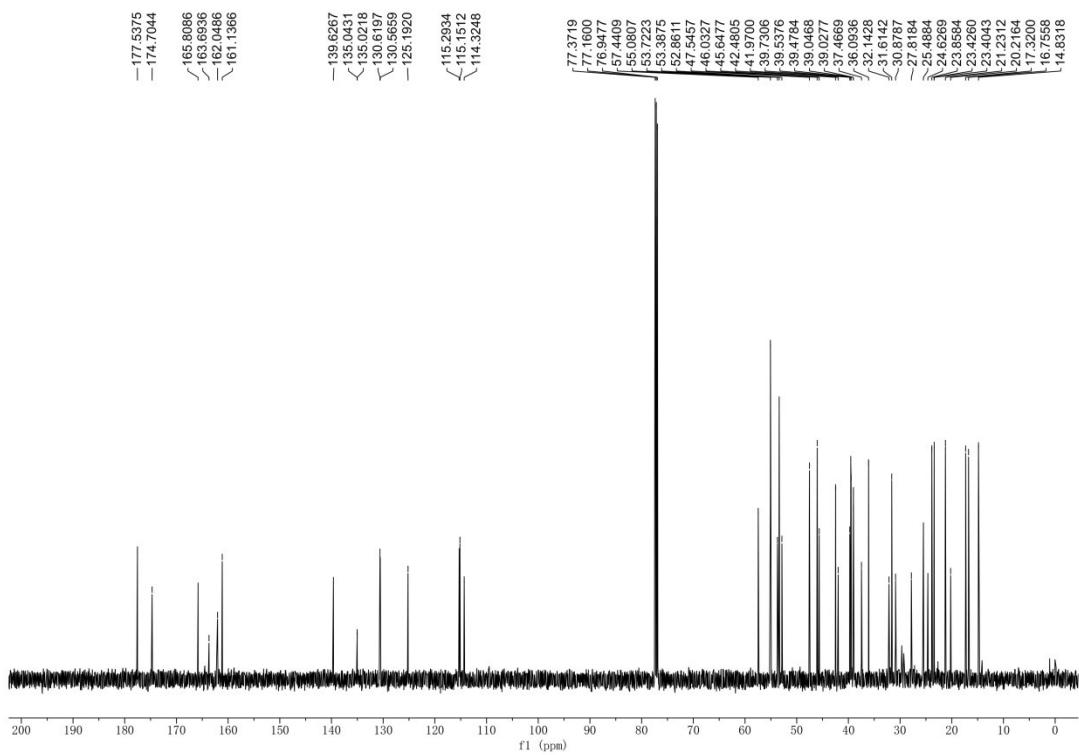


Fig. S71. ^{13}C NMR spectrum of compound 9d (150 MHz, CDCl_3)

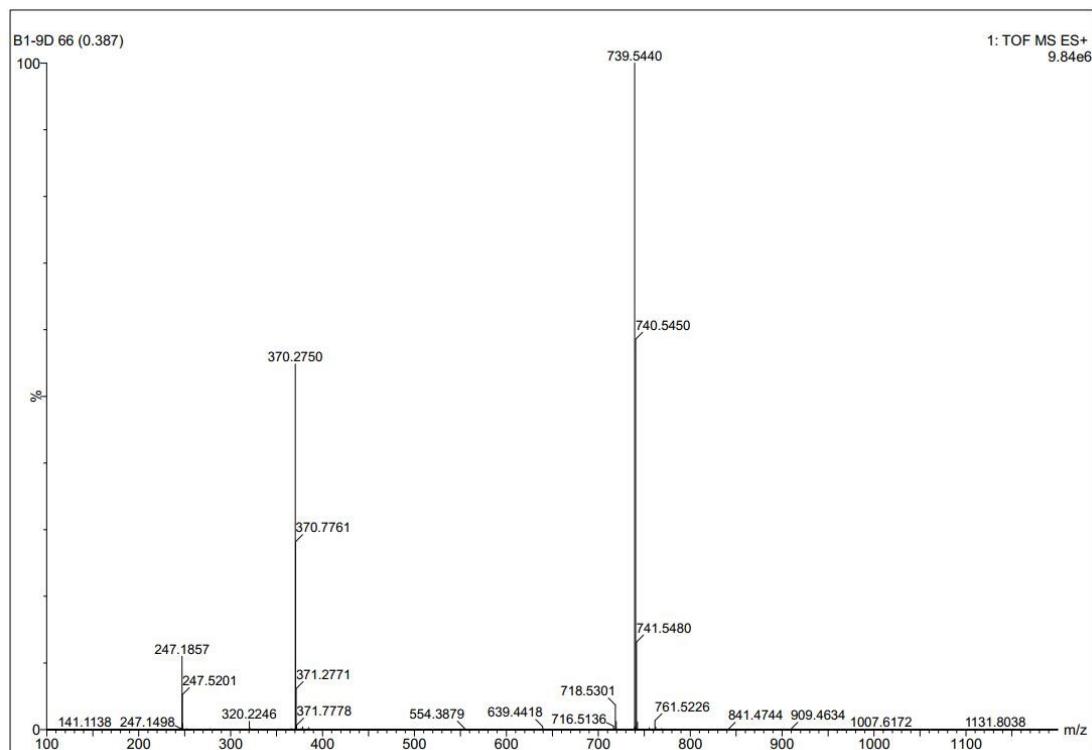


Fig. S72. HRMS spectrum of compound 9d

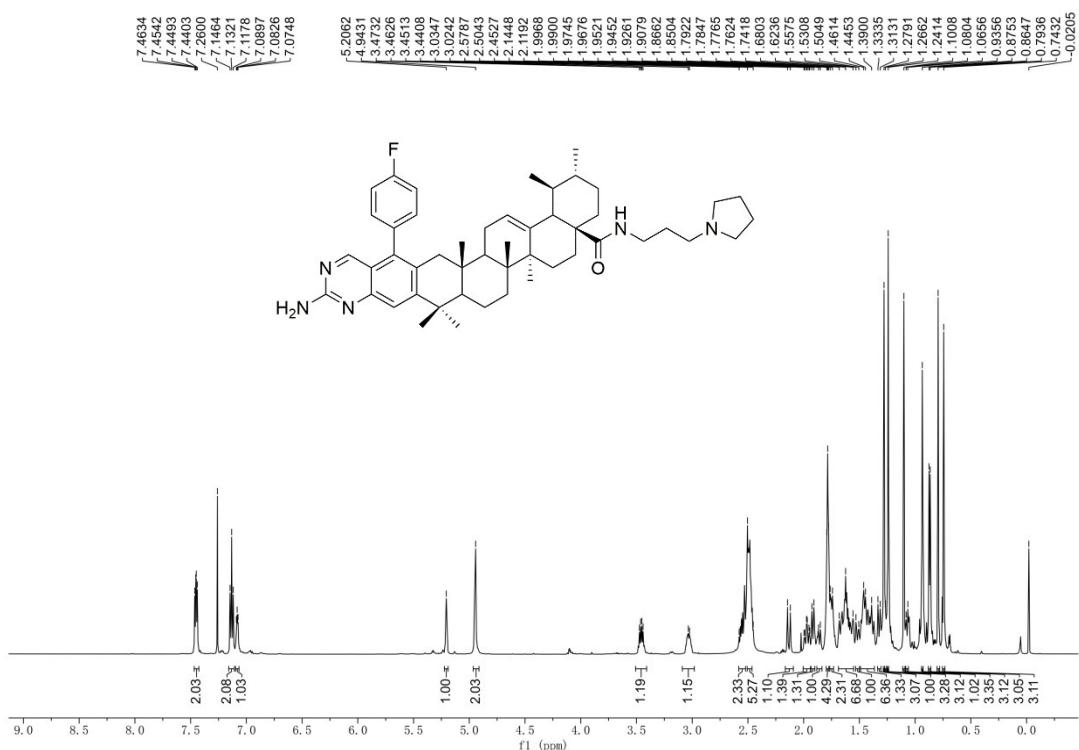


Fig. S73. ^1H NMR spectrum of compound 9e (600 MHz, CDCl_3)

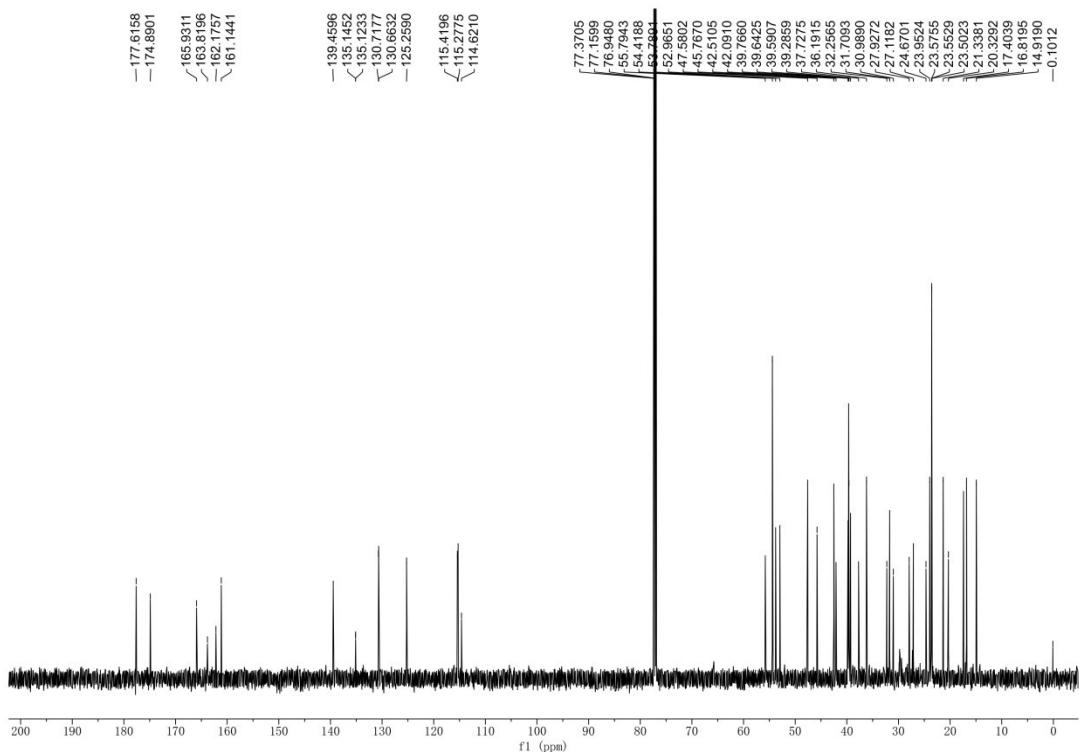


Fig. S74. ^{13}C NMR spectrum of compound 9e (150 MHz, CDCl_3)

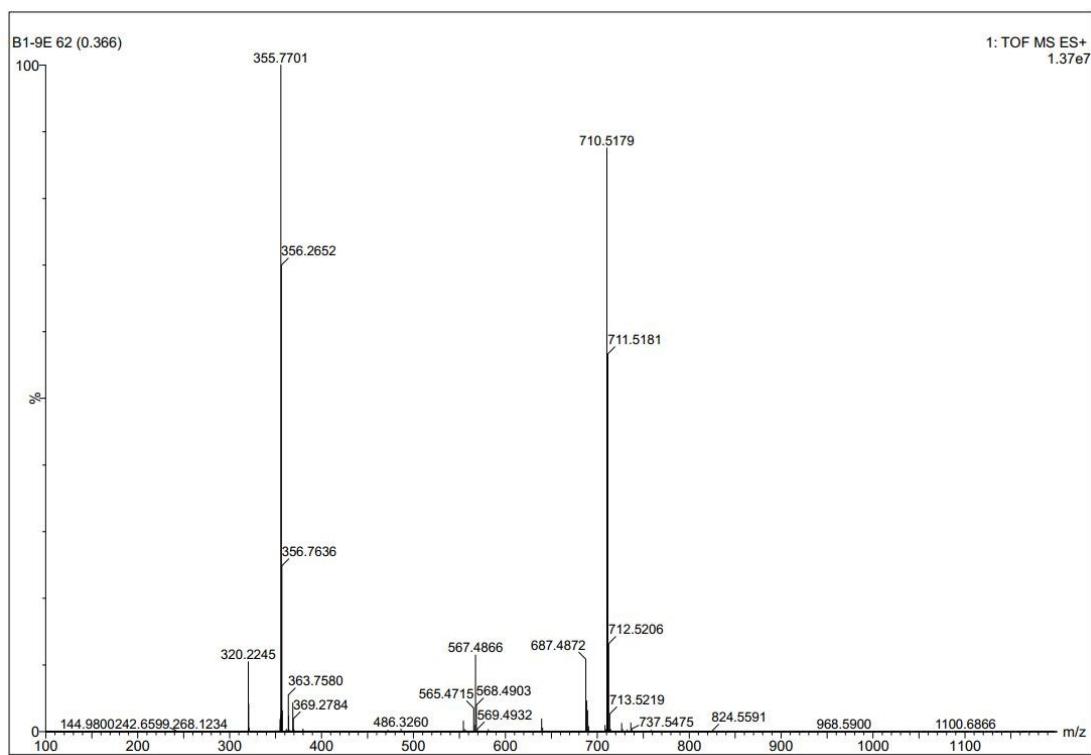


Fig. S75. HRMS spectrum of compound 9e

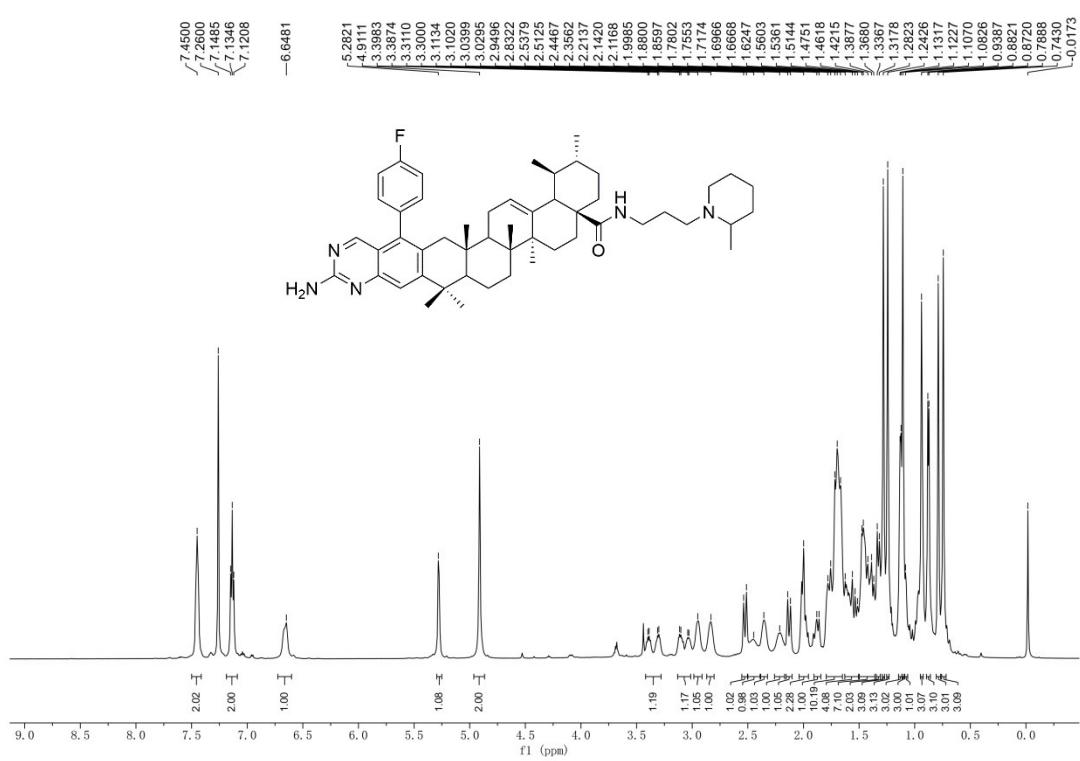


Fig. S76. ¹H NMR spectrum of compound 9f (600 MHz, CDCl₃)

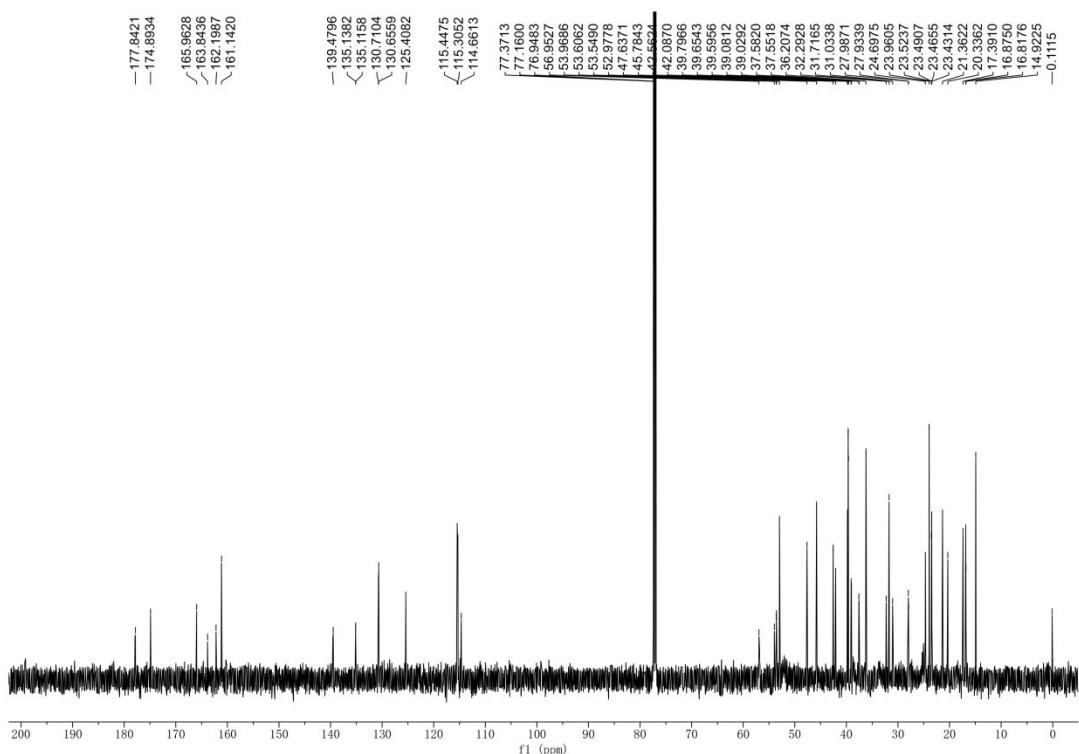


Fig. S77. ^{13}C NMR spectrum of compound 9f (150 MHz, CDCl_3)

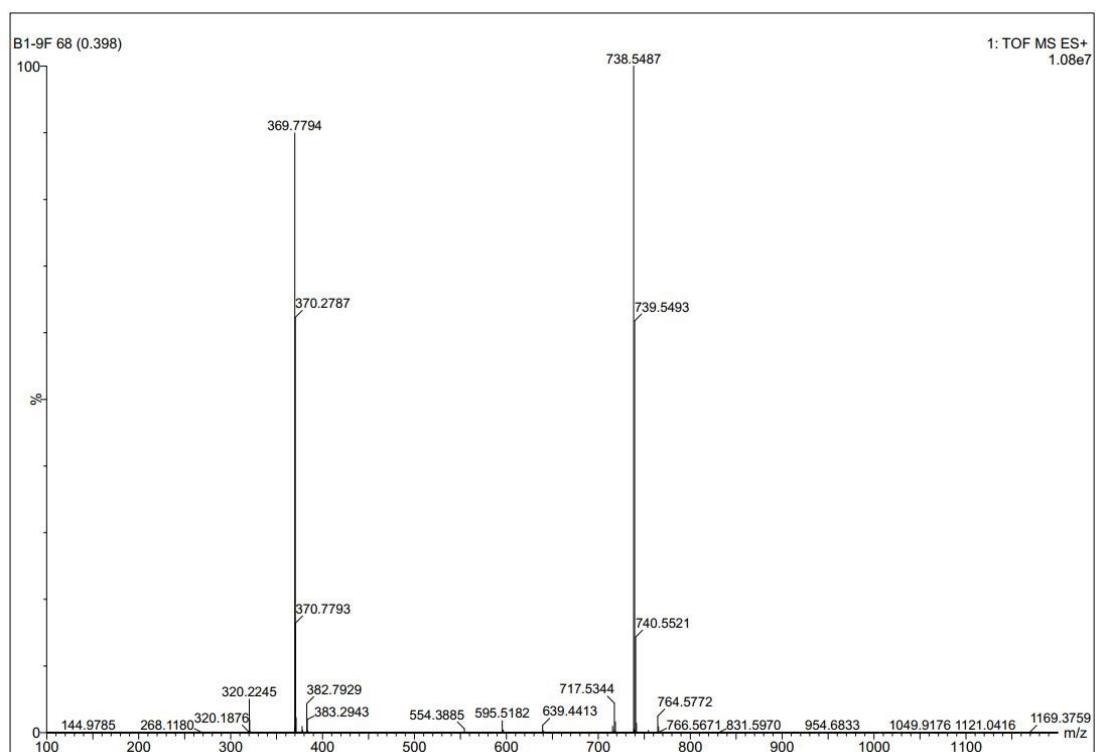


Fig. S78. HRMS spectrum of compound 9f